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New Sampling Theory for Measuring Ecosystem Structure

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Results of the research project included a definition for the bandwidth of an ecosystem in the frequency domain, an indication of the effect of measurement noise on the sample period for data acquisition, a scheme for reducing this noise, and a computer code for model identification based upon the experimental design developed. The project also produced the conditions under which two new schemes for model identification were applicable to the construction of linear compartment models. These new identification schemes were based upon system input perturbations and state observations which were often readily implemented in the laboratory.

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New Sampling Theory for Measuring Ecosystem Structure

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FOREWORD

Environmental protection efforts are increasingly directed towards preventing adverse health and ecological effects associated with compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Environmental Systems Branch studies complexes of environmental processes that affect the transport, transformation, degradation, and impact of pollutants or other materials in soil and water.

This research includes the development and testing of mathematical models that can predict general behavior of toxic organic materials in terrestrial and aquatic ecosystems. The sampling theory and related systems analyses in this report combine model development with preliminary testing using small laboratory ecosystems. This method represents an explicit procedure for designing laboratory ecosystem experiments that provide appropriate tests of model validity.

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ABSTRACT

This research considered the application of systems analysis to the study of laboratory ecosystems. The work concerned the development of a methodology which was shown to be useful in the design of laboratory experiments, the processing and interpretation of the results of these experiments, the development of model structures for microcosms based upon experimental data, the testing of the predictive capabilities of evaluative models, and the analysis of measurement errors in the presence of noise. Development of the experimental design methodology was based upon a non-Nyquist sampling theory which gave *a priori* computable bounds on the sample period for data collection.

Results of the research project included a definition for the bandwidth of an ecosystem in the frequency domain, an indication of the effect of measurement noise on the sample period for data acquisition, a scheme for reducing this noise, and a computer code for model identification based upon the experimental design developed. The project also produced the conditions under which two new schemes for model identification were applicable to the construction of linear compartment models. These new identification schemes were based upon system input perturbations and state observations which were often readily implemented in the laboratory.

The research objective was to produce a scheme for the evaluation of microcosm models used for the assessment of the environmental transport, transformation, degradation, and fate of toxic materials in aquatic systems. An hypothesis was advanced that the evaluative scheme will be developed in the near future into a procedure by which models are tested against laboratory data and refined until they realistically represent perturbed natural ecosystems receiving toxic inputs.

The report was submitted in fulfillment of Research Grant R-805564010 by Oklahoma State University under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period October 23, 1977, to October 24, 1978, and the work was completed as of November 1, 1978.

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It is often difficult to distinguish between basic and applied research. And, with respect to the research described in this report, it is often hard to discern the part funded by the EPA grant from that funded as basic research in systems theory by NSF Grant ENG75-05341-A01.

SECTION 1

INTRODUCTION

This research report concerns an investigation into the application of systems analysis to the study of laboratory ecosystems. Despite the recent resurgence of interest in microcosms, there appears to be no clear understanding of how to best use system theory and mathematical modeling in this important research area. However, there is apparently some agreement as to the use of laboratory ecosystems in ecological research. At least with respect to general research objectives important to the U.S. Environmental Protection Agency, the following reasons for microcosm research are mentioned by Draggan (1976), Brockway, et al. (1978) and Van Voris, et al. (1978): (1) to develop a screening method capable of assessing the environmental fate and effect of chemicals, (2) to study basic ecosystem processes under controlled environmental conditions, (3) to study ecosystem level variables as measures for ecological complexity, and (4) to test or verify mathematical models.

The appeal for microcosm studies is presumably based upon the replicability of experiments which can be performed. This replicable nature of microcosm experiments is generally assumed to result from the control which can be exerted over the laboratory environment. Thus, an ecologist concerned with the study of ecosystem function can employ the hypothesis that microcosms subjected to similar physical and chemical conditions, even when inoculated with samples derived from different sources, will develop into functionally similar systems, see Brockway, et al. (1978). Two quantitative tools are required for work based upon this hypothesis of functional invariance: (1) a rigorous experimental design for measuring ecosystem structure and (2) a theoretical construct which relates ecosystem structure and function. The research reported on here presents the idea that system theory and mathematical modeling can provide both of these tools.

There are also diverse opinions on how to interpret or apply the results of microcosm research. Many ecologists view microcosms as "stripped down" or "simplified" biological models which are intended to simulate some specific natural process (Odum, 1971, p. 21). On the other hand, Brockway, et al. (1978) view laboratory ecosystems neither as biological models nor as analogs of natural ecosystems. Instead, they take what may be a more realistic viewpoint that microcosms are ecosystems in their own right which have their own community structure, mineral cycling, and pathways for energy flow typical of all natural systems. It can be expected that toxic material would disrupt such integrated microcosm processes in a manner similar to any other ecosystem of related structure and function. Thus, a mathematical model which is designed to predict the fate and effect of a substance in any ecosystem which represents a class of systems defined by specific functional attributes should at least be capable of similar predictions for a microcosm belonging to the same class. It follows that models developed for screening can be tested in the laboratory against replicable results derived from perturbed microcosm

experiments provided a rigorous theory for sampling ecosystem structure is employed for data acquisition. Within the arithmetic precision of the experimental data acquired from the microcosm, such a theory for sampling ecosystem structure must completely capture the inherent dynamics of the mathematical model. Thus, the use of system analysis is employed to help insure the results of microcosm experiments are useful in testing the prediction of ecological fate and effect made by mathematical models.

The idea that systems analysis has application to microcosm research is not new. System applications usually focus on the use of models to explore potentially interesting microcosm experiments, the testing of models against microcosm data, and the use of basic model structure to define what variables are of interest and hence what should be measured. The last potential use mentioned may hint at the most important application for system analysis, i.e. its use in the design of experiments. Mulholland and Gowdy (1977) presented, for perhaps the first time, the concept that systems analysis and modeling can be used to develop a quantitative theory for measuring ecological structure in laboratory microcosm. The idea is to use systems analysis, in much the same way statistics is now used, to design microcosm experiments. Starting with a theory used to produce bounds on the temporal sampling period for measuring compartment level variables in a microcosm, research during the past year has produced a design for input function which places in evidence the complete dynamic response resulting from a system level perturbation. The resultant experimental design provides for the collection of sufficient data to identify the parameters of two models types: (1) a sequence of (local) linear models with *a priori* unconstrained structure and (2) a nonlinear model of postulated, but not quantified, structure. The basic input function design also allows for the collection of independent data useful in testing the responses of the resultant models to perturbations.

In summary, research has disclosed an experimental design for laboratory ecosystems which provides a method for introducing the appropriate system level perturbations, introduced through natural system input ports, in order to elicit full system dynamic response. The design also provides for amplitude calibration and periodic time sampling which captures the full dynamic state response. The state response data which result from the experimental design establish a test for system linearity with respect to multiple perturbations, a data base for constructing local linear models, an independent data base for nonlinear model construction, and still another data base for testing model response.

SECTION 2

CONCLUSIONS AND RECOMMENDATIONS

The results of this research have produced an experimental design for the laboratory analysis and evaluation of perturbed microcosms. The complete design has not yet been tested against actual experiments. A continuation of this line of research would allow such a test to take place. Additional research is also needed for the development of a stochastic version of the experimental design, thus combining statistics with systems analysis which could lead to a powerful technique for error analysis. The development of a statistical error analysis should give rise to techniques for filtering raw data, and hence for minimizing measurement errors in the presence of noise. Testing of mathematical models against microcosm derived data, based upon the proposed development of a stochastic experimental design, could lead to a rigorous methodology for model validation.

With respect to analysis in the frequency domain this research has been unable to reconcile the Mulholland-Gowdy sampling theory with the Nyquist theory used in engineering systems analysis. The main problem here, yet to be resolved, concerns the development of an effective technique for bandlimiting ecosystems. Unlike engineering systems, it may be impossible to define a useful measure for the equivalent bandwidth of an ecosystem. The Mulholland-Gowdy sampling theory provides bounds on the sample period used for data collection in the laboratory, which in turn describe a window in the frequency domain where the state response spectrum resides. However, it is unclear whether or not this window, having been developed under prescribed input conditions, gives a universal representation for the frequency spectrum of an ecological system.

The study of two special forms of compartmental structure has produced a generalization of the concept of identifiability. First, for systems, in which the state is not directly observable, but measurements of only accumulation pools are possible, the conditions for identifiability, controllability and observability have been defined. Second, the conditions under which systems receiving a constant infusion of labeled material are identifiable have been produced. Although these conditions on the identifiability for the constant infusion method are somewhat limited by system structure, it should be noted that most system scientists believe that systems cannot be identified from only steady-state data and that excitation of transient states are always required. In spite of this misconception, it has been shown that complete sets of model parameters can be obtained when systems are in steady-state under specific conditions which are often met in practice. The study of identifiability conditions is necessarily theoretical in nature. So, in order to be of some use in experimental design, the conditions which have resulted from this research must be tested in the laboratory against the data derived from microcosm experiments.

SECTION 3

SAMPLING THEORY AND APPLICATIONS

MODEL IDENTIFICATION

The determination of a model relating structure and function of a system from experimental time series observations of the state is known as system identification. It includes the estimation of system parameters for the observable components within the biological system. One of the fundamental problems of system identification is whether or not the parameters can be determined uniquely (Lee, 1964). If unique estimates cannot be obtained (the system is not identifiable), then the experimental procedures should be altered. Determination of structure from function results from an input-output tracer experiment. The different identification schemes that are available can be classified according to the basic elements of the problem and the input signals, the earliest methods being those based on frequency, step and impulse responses. Special inputs rather than those of normal operation are necessary for these schemes, so the techniques are termed off-line identification and therefore apply only to linear stationary processes where input/output relations which hold for one set of inputs are good for all inputs (Graupe, 1972).

For the purposes of tracer analysis the local model is a linear donor controlled biological compartment model defined by

$$\dot{\underline{x}} = \underline{A}\underline{x} + \underline{B}\underline{u} \qquad (3.1)$$

where the state $\underline{x}$ is an n-dimensional vector of the compartmental contents, the coefficient matrix $\underline{A} = (a_{ij})$ is an ordered array of the compartmental rate coefficients, the input $\underline{u}$ defines the ecosystem inputs as an m-dimensional vector, and the input connection matrix $\underline{B} = (b_{ij})$ is of n rows and m columns with entry b_{ij} equal to one if input u_j enters compartment i, if not, the entry is zero.

In equation (3.1), the inputs $\underline{u}$ and their entry into the ecosystem compartments, the $\underline{B}$ matrix, are known. The solution of the identification problem for (3.1) requires a method to determine the entries in $\underline{A}$, containing the rate coefficients, given sufficient measurements of the state $\underline{x}$.

BASIC EXPERIMENT

The use of radioactive tracers is prone to varying experimental procedures, especially with the advent of highly sophisticated instruments and new radioisotopes. Practical experiments must be designed to coexist with developed theoretical techniques. A standard method has developed using three basic experiments to assess the environmental impact on aquatic microcosms of

toxic material inputs. As shown in Table 1, the first test input represents a slug of toxic material, the second considers a constant chronic input level of toxin, and the third forms the superposition of the aforementioned experiments. The microcosm responses to the three basic inputs are also shown in Table 1. The toxic slug of part (a) elicits a transient response with initial condition x_o, and the constant input level of part (b) gives rise to a steady-state defined by x_s. By assuming a linear model for the microcosm system, part (c) of Table 1 illustrates the resultant superposition principle. It should be noted that the basic microcosm experiments contain information regarding the validity of the linear modeling assumption. For linear models, the microcosm responses to the inputs of Table 1, parts (a) and (b), should sum to give the response to the input of part (c). If this superposition is in fact true, the single dose method [the input of part (a)] can be effectively used to identify the numerical model for the microcosm. Therefore, the validity of the linear state model (3.1) should be clear from the outcomes of the basic experiments of Table 1. Generally, a local linear model can be identified for small perturbations (x_o is small compared to x_s) caused by impulse inputs at a given system loading defined by u_o. A local model defined in this way will be dependent upon the system loading.

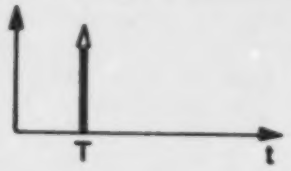
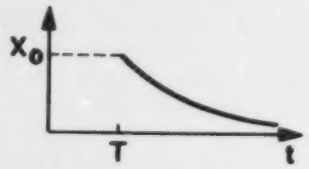
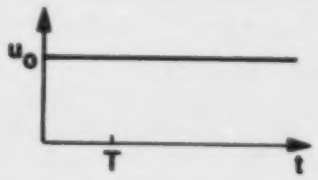
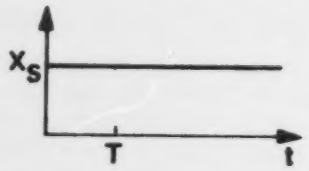
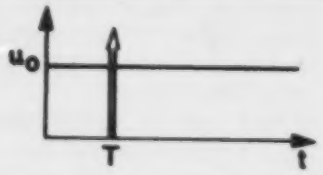
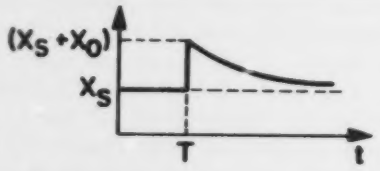
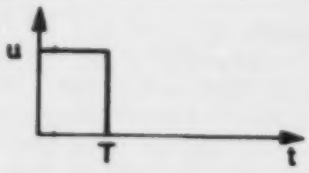
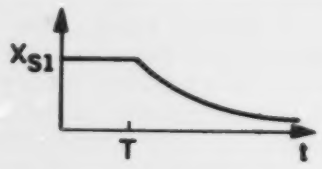
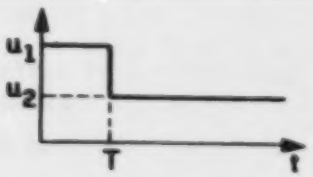
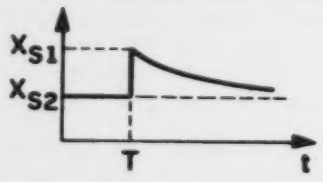
Also in Table 1, two new experiments are proposed for linear model identification using tracers or toxic material flows as microcosm inputs. These inputs, based upon step functions, have been designed for ease of application in the laboratory and mathematical convenience for system identification. These basic experimental inputs lead to a sampling theory which is essential to the successful application of standard identification schemes. This result, in turn, prescribes an experimental design for the *a priori* determination of the period for data collection in the laboratory.

The basic experiment of part (e) of Table 1 has been designed as an identification technique for local linear models. Linearity can be tested in the laboratory by observing response superposition as result of adding two microcosm inputs.

As previously noted, the basic experiments (d) and (e) of Table 1 have been designed for ease of application in the laboratory and to aid in the development of a sampling theory. It turns out that under certain conditions these basic experiments also avoid the problem of tracer analysis of having input access to each compartment. However, the equivalence between the inputs of parts (c) and (e) of Table 1 is essential in eliminating the so-called precursor problem. In Figure 1 an example of a two compartment model with a single dose input into the precursor compartment is shown in part (a) along with the input and compartment response plots in part (b).

The precursor problem deals with the impossibility of estimating the maximum value (x_m) of the response of compartment x_2 to the impulse input to compartment x_1. In order to develop an effective laboratory data collection strategy, it is necessary to have known rules for amplitude and time discretization. Because x_m is known before the experiments is completed, it is very difficult in ordinary tracer analysis to develop a rule for amplitude quantization. Given a sample period, data on microcosm structure is collected at discrete times and the values of these data are quantized by the finite arithmetic precision of the measuring instruments. However, the quantization of

TABLE 1. BASIC MICROCOSM EXPERIMENTS

	Input	Response
(a)		
(b)		
(c)		
(d)		
(e)		

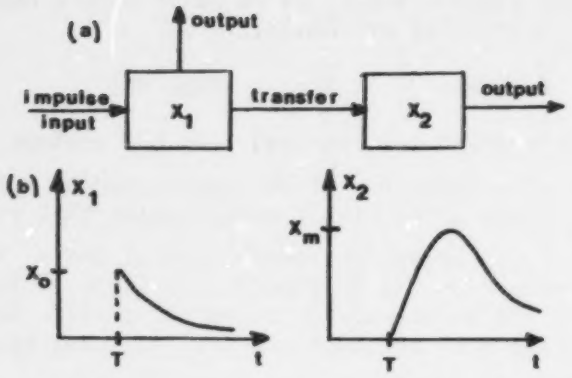


Figure 1. An example two compartment system with precursor.

time and amplitude are not sequential processes; they are, in fact, related to one another. This gives rise to the commonly used laboratory procedure for single dose experiments of taking microcosm samples very rapidly at first until x_2 reaches its maximum and then more slowly to accommodate the compartmental dynamics inherent in the free response. The asynchronous sampling procedure described is difficult to analyze, particularly when the propagation of measurement errors through the identification algorithm is required. A periodic sampling scheme would be more desirable.

The basic experiments (d) and (e) of Table 1 eliminate the precursor problem. This follows from the fact that transitions between steady-states in compartmental system are monotonic and bounded by the initial and final states (Thron, 1972). Therefore, the amplitude quantization process is well defined, and a periodic sampling strategy is possible.

SAMPLING THEORY

The collection of time series data for each compartment $x_i(t)$ in the biological system takes place in two distinct steps in which first time and then amplitude are quantized. The samples of the state are obtained only at discrete times. These samples are periodically spaced apart by τ time units giving a data base defined by $\{\underline{x}(0), x(\tau), \ldots, x[(k+1)\tau]\}$. It has been shown that the minimum data base for solution of the identification problem is (n+1) state samples or k = n. Next, the finite precision with which the measurements of state are made must be accounted for in terms of a mathematical relationship. The assumption is that $x_i(t)$ and its samples are fixed point numbers which are less than or equal to one. These samples, arising from radiological measurement equipment, are data with no more than a fixed number of digits to the right of the decimal point. Let 10^{-d}, where d is a positive integer, be the smallest non-zero number in the data set.

Because the eigenvalues of the system described by (3.1) are bounded by Gerschgorin circles of known radii (Hearon, 1963), it is not difficult to show that transitions between steady-states, as in Table 1, are bounded by two exponential factors (see Mulholland and Gowdy, 1977):

$$\exp(-\alpha t) \leq x_i(t) \leq \exp(-\delta t) \tag{3.2}$$

where $\alpha/2 = T_o^{-1}$ is the maximum turnover and δ is the minimum non-zero transfer out of the system. The selection of the sample period τ for data collection is now possible. Using (3.2), it is easily shown that τ is bounded by $\tau^- \leq \tau \leq \tau^+$, where τ^+ is the maximum sample period and τ^- is the minimum, both of which are determined by the arithmetic precision of the state samples.

It is possible for the sample period to be too small. This occurs when $x_i(t)$ and $x_i(t+\tau)$ have the same arithmetic precision; that is, when $x_i(t+\tau)$ is truncated to d digits, it equals the truncated value of $x_i(t)$. Since (3.2) gives an upper bound for $x_i(t)$, a measure of the minimum sampling time, denoted by τ^-, is given by

$$1\text{-}10^{-d} = \exp(-\delta\tau^-) \leq x_i(\tau^-) \tag{3.3}$$

or solving for the minimum sampling period yields

$$\tau^- = (-1/\delta)\ \ln\ (1\text{-}10^{-d}). \tag{3.4}$$

If $\tau > \tau^-$ the state samples are independent, but an upper bound on τ exists. Suppose τ is chosen large enough so that $x_i(n\tau)$, the last sample in the data set, is truncated to zero, then the data set is incomplete and the identification problem cannot be solved. Thus, the maximum sample period, denoted by τ^+, must be such that the (n+1)-th sample is at least equal to the smallest number in the finite precision arithmetic; that, $x_i(n\tau^+) \geq 10^{-d}$. But (3.2) gives a lower bound for $x_i(t)$; thus, the maximum sample period is easily computed from

$$10^{-d} = \exp(-\alpha n\tau^+) \leq x_i(n\tau^+), \tag{3.5}$$

which gives

$$\tau^+ = (-1/2nT_o^{-1})\ \ln\ (10^{-d}). \tag{3.6}$$

Based upon intuition, experience, isolated laboratory experiments, and/or estimates from the literature, biologists tend to know the turnovers for the compartments present in a system. Such knowledge is at least accurate to an order of magnitude. Thus, the maximum sample period is easily determined from (3.6).

IDENTIFICATION ALGORITHM

Consider the experiment of part (d) of Table 1 in which a constant (known) input is applied to an ecosystem modeled by (3.1). After sufficient time has elapsed, a steady-state is observed, as indicated by $\dot{\underline{x}} = \underline{0}$. Denote this steady-state by the vector $\underline{x}_s$, which is the solution of

$$\underline{0} = \underline{A}\underline{x}_s + \underline{B}\underline{u}. \tag{3.7}$$

In the experiment under discussion, the input is assumed to be a constant rate of infusion of labeled material. It is also assumed the steady-state can be measured using standard radiological methods. On a new time scale, the experiment is re-started at time $t = 0$ by removing all inputs to the ecosystem. Thus, before $t = 0$, the system is in steady-state $\underline{x}(0) = \underline{x}_s$, while for $t > 0$ the state of the system is governed by the solution of

$$\dot{\underline{x}} = \underline{A}\underline{x} \tag{3.8}$$

because $\underline{u} = \underline{0}$ for $t > 0$. The labeled contents of the compartments of the ecosystem start at $t = 0$ with values determined by $\underline{x}_s$ and decrease exponentially as t becomes large as all the labeled material flushes from the system along the pathways for material transfer.

Discretized in time the solution of (3.8) is governed by

$$\underline{x}(i\tau) = \underline{\Phi}\,\underline{x}[(i-1)\tau] \qquad (i = 1, 2, \ldots), \tag{3.9}$$

where $\underline{\Phi} = \exp(\underline{A}\tau)$ with $\tau^- \leq \tau \leq \tau^+$.

A continuous record of the state $\underline{x}(t)$ is not required in order to determine $\underline{\Phi}$, which by definition gives $\underline{A}$. Since $\underline{\Phi}$ is an $n \times n$ constant matrix, constraint equations numbering n^2 are required to prescribe the entires in this matrix. The problem reduces to finding $\underline{A}$ from a finite number of discrete and regularly spaced samples of the state, given at times $t = 0, \tau, 2\tau, \ldots, k\tau$ where τ is the sample period. Substitution of these state samples into (3.9) gives

$$\begin{aligned}
\underline{x}(\tau) &= \underline{\Phi}\,\underline{x}(0) \\
\underline{x}(2\tau) &= \underline{\Phi}\,\underline{x}(\tau) \\
&\vdots \qquad\quad \vdots \\
\underline{x}(k\tau) &= \underline{\Phi}\,\underline{x}[(k-1)\tau].
\end{aligned} \tag{3.10}$$

This linear algebraic system contains n^2 unknowns (all the entries of $\underline{\Phi}$) and k independent vector equations of n components each, for a total of kn equations. For $k < n$ no unique solution of (3.10) exists, and the system is overdetermined for $k > n$. Thus $k = n$ or $(n+1)$ discrete samples of the state are necessary and sufficient to determine $\underline{\Phi}$.

It is possible to rewrite system (3.10) in the following more standard algebraic form

$$\underline{X}_2 = \underline{\Phi}\,\underline{X}_1, \tag{3.11}$$

where $\underline{X}_1$ is an n x k matrix formed by columns from the first k state samples,

$$\underline{X}_1 = \{\underline{x}(0), \underline{x}(\tau), \ldots, \underline{x}[(k-1)\tau]\}, \tag{3.12}$$

and $\underline{X}_2$ is similarly obtained from the next k state samples delayed by one sample period,

$$\underline{X}_2 = \{\underline{x}(\tau), \underline{x}(2\tau), \ldots, \underline{x}(k\tau)\}. \tag{3.13}$$

For k = n in (3.10) the solution for $\underline{\Phi}$ is obtained by inverting the matrix $\underline{X}_1$. This assumes n linearly independent state samples which is indeed the case when the ecosystem model defined by (3.1) applies. Thus, the identification problem is solved by

$$\underline{A} = (1/\tau)\ \ln(\underline{X}_2\underline{X}_1^{-1}) \tag{3.14}$$

under these stated conditions.

It is mathematically necessary and sufficient to make (n+1) discrete state measurements in order to solve for $\underline{\Phi}$. At least (n+1) measurements are required for a unique solution, however on occasion it may be desirable to obtain more than (n+1) state samples. For example, when significant experimental error is suspected in the state data, it may be of use to increase the dimension of the data set beyond (n+1). Under these conditions k > n, and there are more equations than unknowns in (3.10). A Gaussian least squares estimate for the solution of $\underline{A}$ can then be obtained (Lee, 1964).

SIMULATED EXPERIMENT

Early in the project, it was surmized that problems might arise in getting the data from the EPA planned microcosm experiments which were designed to test the Mulholland-Gowdy sampling theory. So, a simulation of experimental data was devised using an ecosystem model. It is difficult to theoretically analyze the propagation of data noise through a nonlinear algorithm. Since the identification algorithm is nonlinear, a simulation was used to examine the effects of data noise errors (on the algorithm). In the simulations, data noise was propagated through the algorithm to obtain the statistics of individual parameters within the identified model.

The identification algorithm, defined by (3.11), requires discrete samples of the system state: $\underline{x} = \underline{x}(k\tau)$. Actually, the ensemble of these samples is itself a sample function for a stochastic process. Because of noise inherent in the microcosm processes and errors introduced by the measurement techniques and instruments, the analysis of the basic experiment (defined in Table 1) cannot be wholly based upon deterministic systems theory, but it must include a statistical analysis. The statistical interpretation of the basic microcosm experiment relies upon the fact that the initial and final steady-states are random variables with measurable statistics. These steady-states are connected by a sample function of a stochastic process which is a statistical repre-

sentation of the sequence of transition states.

The stochastic process which represents the transition states has been simulated by a deterministic variable ($\underline{z}_k$) perturbed by a uniformly distributed random variable ($\underline{w}_k$).

$$\underline{x}_k = \underline{z}_k + \underline{w}_k \tag{3.15}$$

for each k = 0, 1, ... , n. The motivation for this representation derives from knowing (by measurement) the system state to an arithmetic precision of 10^{-d}. Then, the random variable $\underline{w}_k$ is uniformly distributed from 0 to 10^{-d} with a probability density function given by Figure 2. This perturbation simulates noise superimposed upon the truncated state.

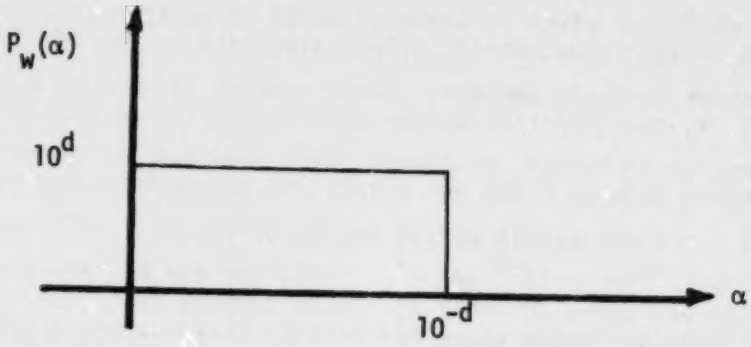


Figure 2. Probability density function for $\underline{w}_k$.

The solution of (3.11) for the identified model shows in (3.14) a dependence upon the sample period. Indeed, there probably exists an optimal sample period which depends upon the statistics of the experiment. In order to test for this optimal sample period and in general study how noise propagates through the identification algorithm to the entries in the model $\underline{A}$-matrix, a Monte Carlo experiment was decided upon. The exact solution of the model, correct to d-digits, has been obtained. The state is then truncated to d-digits and corrupted by noise according to (3.15). Simulated noise measurement data, defined by (3.15) are passed through the identification algorithm many times until the statistics of the entires in the $\underline{A}$-matrix are measureable. The following example will clarify this scheme.

The ecosystem model chosen to represent, through computer simulations, the effect of measurement noise on the identification algorithm and sampling theory is a hypothetical ecosystem first described by Smith (1970). Smith's system is not a model of a real system, but is a model built upon realistic numerical parameters and a state response which mimics an aquatic ecosystem operating under a phosphorus loading. Very simply, Smith's system consists of three compartments: water (x_1), an aquatic plant population (x_2), and an herbivore population (x_3). The only ecosystem input (u_1) is the phosphorus contained in the water flowing through the system. The outputs are phosphorus from the water compartment and from the herbivore compartment due to emigration or emergence. The plants exchange phosphorus with the water compartment,

which is transferred to the herbivores through grazing.

From data presented by Smith, the rate coefficients can be computed, which results in

$$\begin{aligned} \dot{x}_1 &= 5x_2 + 5x_3 - 16x_1 + u_1 \\ \dot{x}_2 &= 14x_1 - 95x_2 \\ \dot{x}_3 &= 90x_2 - 14x_3 \end{aligned} \tag{3.16}$$

as a (local) linear donor controlled model defined near the prescribed input of u_1 = 100 mgP/day. The time scale of the model is defined by the rate coefficients which are given in terms of units of reciprocal days.

With u_1 = 100, equation (3.16) was simulated on the IBM-370 using the CSMP simulation language package. State samples correct to 4 1/2 decimal places, i.e. x_2 takes initial values with 5 significant digits but it eventually declines to 4 signigicant digits, were obtained for 20 different sample periods ranging between 0.005 and 0.120. It should be noted that (3.16) with α = 190 and δ = 2 has sample period bounds of $\tau^- = 5 \times 10^{-6}$ and $\tau^+ = 0.0202$ for d = 5, and $\tau^- = 5 \times 10^{-5}$ and $\tau^+ = 0.016$ for d = 4. For τ = 0.01, the four state samples are given in Table 2. These samples illustrate the particular basic experiment performed where the initial steady-state entrained by the constant input is the initial condition. The input is then removed and the state declines, according to the system dynamics, monotonically to zero.

TABLE 2. TRUNCATED STATE SAMPLES FOR τ = 0.01

k	x_1	x_2	x_3
0	9.5000	1.4000	9.0000
1	8.5748	1.3506	8.9844
2	7.7807	1.2549	8.9052
3	7.0939	1.1519	8.7513

A pseudo-random number generator was then used to drive the Monte Carlo simulations for model identification. The density function for $\underline{w}_k$, uniformly distributed from 0 to 10^{-4}, gives a mean $\mu_w = 5 \times 10^{-5}$ and a variance of $\sigma_w^2 = 8.33 \times 10^{-10}$. Using standard statistical tests with a level of significance of 0.05, it was determined that 400 samples were required to estimate

the mean and variance for $\underline{w}_k$. It was then assumed that 400 computer runs of the identification algorithm were sufficient.

For each sample period, the random number $\underline{w}_k$ was added to the simulated states $\underline{z}_k$ to form the measured data $\underline{x}_k$ for the identification algorithm. A total of 400 models were generated for each τ. Using the estimates given by

$$\hat{\mu}_a = (1/N) \sum_{i=1}^{N} a_i \qquad (3.17)$$

and

$$\hat{\sigma}_a^2 = (1/N-1) \sum_{i=1}^{N} (a_i - \mu_a)^2 \qquad (3.18)$$

for N = 400, the mean and variance for the a_{11} and a_{12} entries in the $\underline{A}$-matrix of (3.16) were determined.

A chi-squared fitness test was performed to test for normality of the distributions for a_{11} and a_{12}. The results are given in Tables 3 and 4.

Spectral plots of $\hat{\mu}_a$ and $\hat{\sigma}_a^2$ for a_{11} and a_{12} appear in Figures 3 through 6. For this particular model ecosystem, the empirical data suggest bounds of 0.007 and 0.07 for the sample period τ as compared to $\tau^- = 5 \times 10^{-6}$ and $\tau^+ = 0.02$ as computed from the theory for d = 5. Bounds for τ cannot be specified more closely because of the statistical nature of the data. For example, the estimated mean for a_{11} is always within acceptable limits of the true value of $a_{11} = -16$ (see Figure 3) regardless of the sample period and independent of the estimated variance. Therefore, the error inherent within the identification algorithm cannot be exactly specified. However, the spectral plots indicate a relationship exists between the sample variance and the sample period. It is possible that future research efforts will disclose a statistical theory for this relationship.

Finally, a comment on the apparent disagreement between the theoretical sample period bounds and those derived empirically from this specific example seems to be in order. The theoretical bounds given in (3.4) and (3.6) are general bounds for all compartmental systems with maximum turnover of $\alpha/2 = 95$ and minimum non-zero exogenous turnover of $\delta = 2$, and that these bounds are exceeded for a specific model does not invalidate the theory. Indeed, a sample period chosen less than $\tau^+ = 0.02$, say $\tau = 0.01$, appears to be perfectly acceptable for model identification.

TABLE 3. CHI-SQUARED TEST FOR a_{11} WITH N = 400 AND 17 DEGREES OF FREEDOM $\chi^2_{17;0.05} = 27.59$

τ	$\hat{\mu}_a$	$\hat{\sigma}_a^2$	α(chi)
.005	-16.024	1.39×10^{-2}	32.4
.006	-15.973	7.90×10^{-3}	31.4
.007	-15.964	4.98×10^{-3}	36.2
.008	-16.057	3.43×10^{-3}	35.3
.009	-16.039	2.51×10^{-3}	41.7
.010	-16.010	1.95×10^{-3}	41.2
.011	-16.010	1.57×10^{-3}	31.1
.012	-15.983	1.31×10^{-3}	25.7
.013	-16.022	1.12×10^{-3}	23.6
.020	-16.016	6.38×10^{-4}	8.2
.030	-15.992	6.39×10^{-4}	7.0
.040	-16.050	9.89×10^{-4}	13.7
.050	-15.997	1.86×10^{-3}	25.2
.060	-15.965	3.95×10^{-3}	10.8
.070	-16.007	9.67×10^{-3}	15.1
.080	-15.780	2.02×10^{-2}	20.9
.090	-16.249	2.14×10^{-2}	6.8
.100	-16.190	3.40×10^{-2}	14.5
.110	-16.178	5.57×10^{-2}	19.7
.120	-16.368	9.33×10^{-2}	55.7

TABLE 4. CHI-SQUARED TEST FOR a_{12} WITH N = 400 AND 17 DEGREES OF FREEDOM $\chi^2_{17;0.05} = 27.59$

τ	$\hat{\mu}_a$	$\hat{\sigma}_a^2$	α(chi)
.005	5.147	2.655	27.2
.006	4.793	1.194	23.3
.007	4.541	0.627	20.6
.008	5.578	0.372	19.2
.009	5.404	0.241	21.2
.010	5.035	0.168	18.2
.011	5.184	0.124	16.5
.012	4.888	0.096	16.9
.013	5.165	0.077	13.9
.020	5.113	0.033	5.7
.030	4.947	1.028	20.8
.040	5.322	0.040	14.3
.050	4.984	0.076	22.8
.060	4.786	0.145	14.4
.070	5.046	0.345	12.5
.080	3.680	0.701	19.5
.090	6.516	0.781	9.1
.100	6.160	1.262	12.9
.110	6.081	2.096	17.7
.120	7.306	3.485	45.1

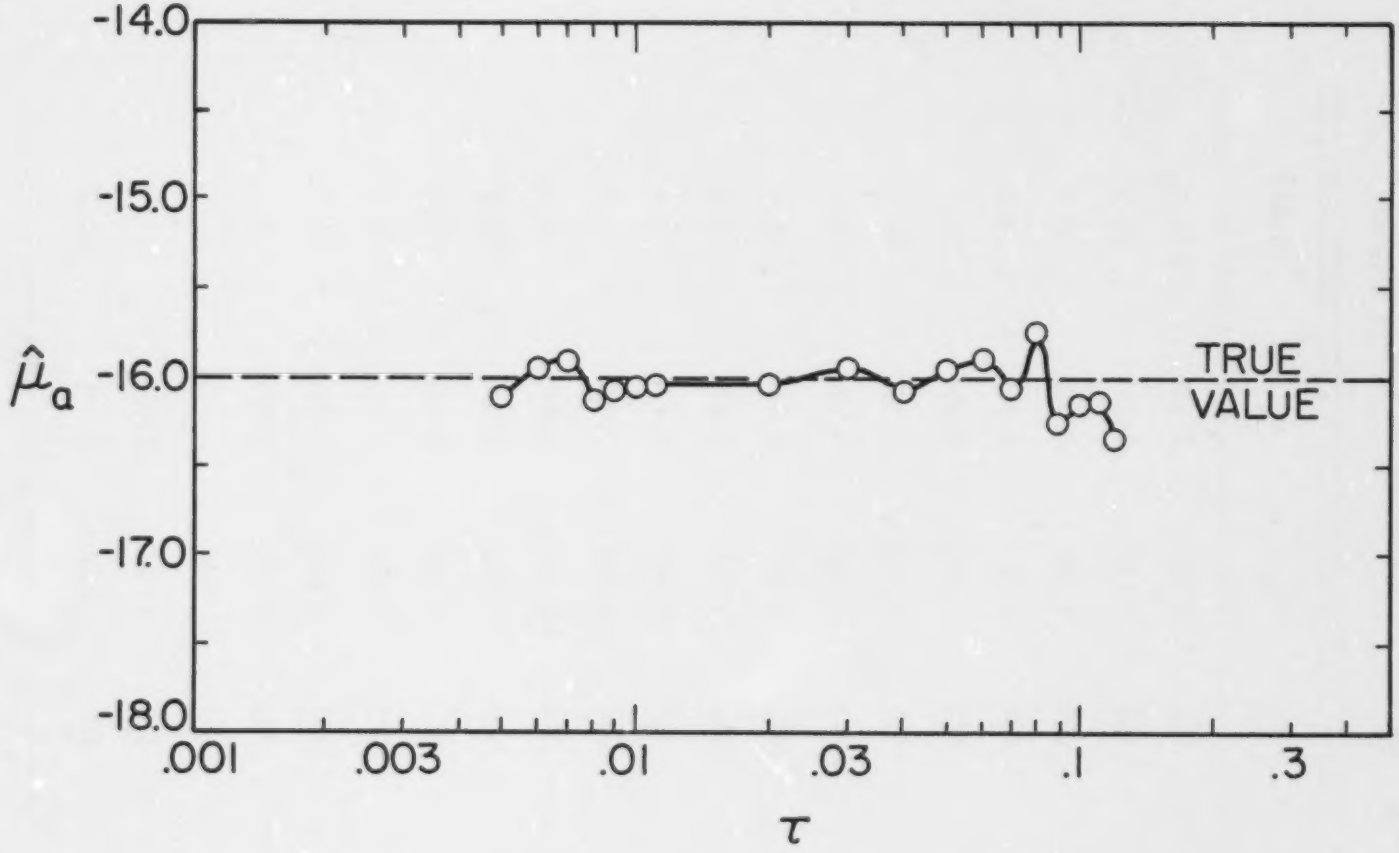


Figure 3. Spectral graph of the estimated mean value for a_{11} of Smith's model.

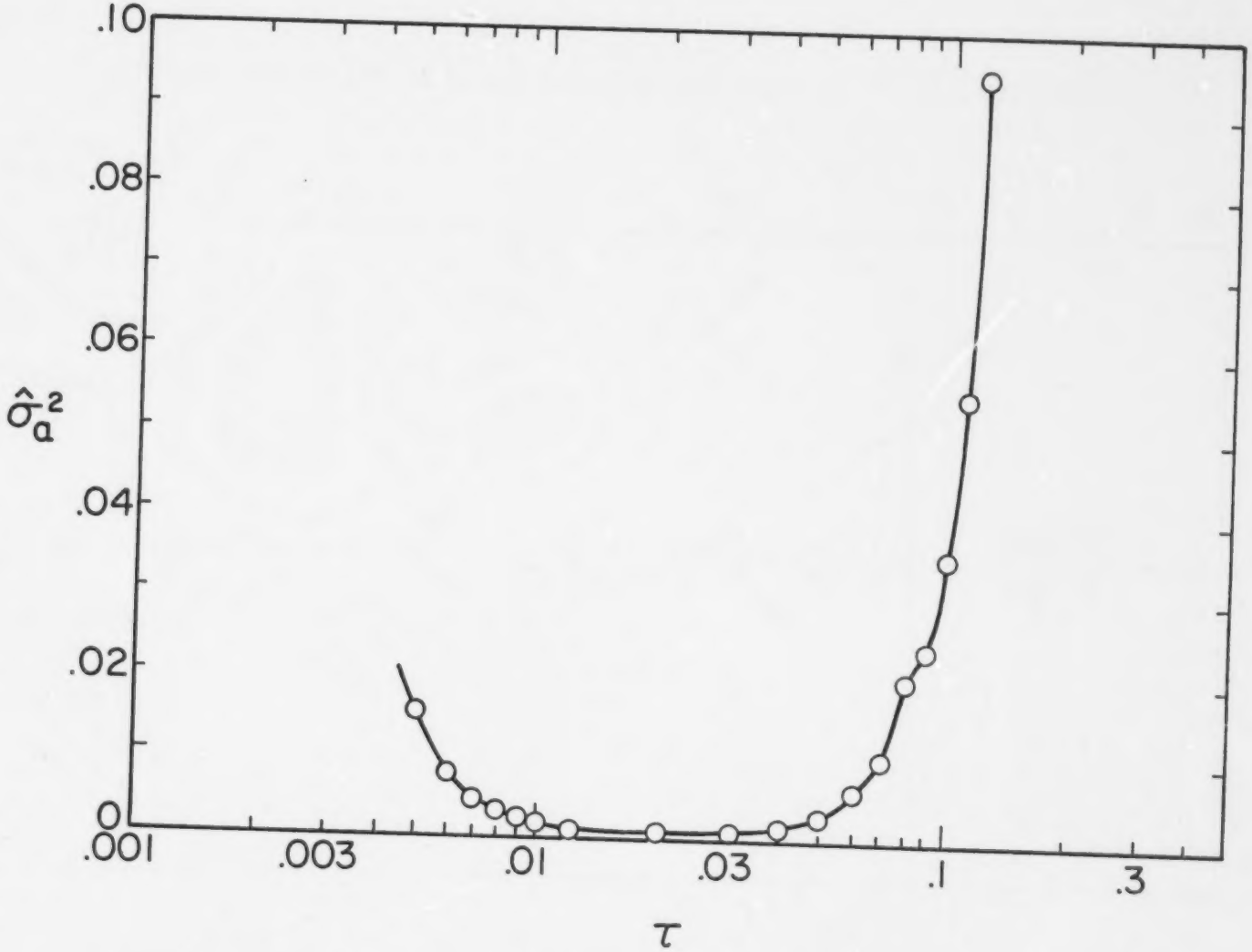


Figure 4. Spectral graph of the estimated variance for a_{11} of Smith's model.

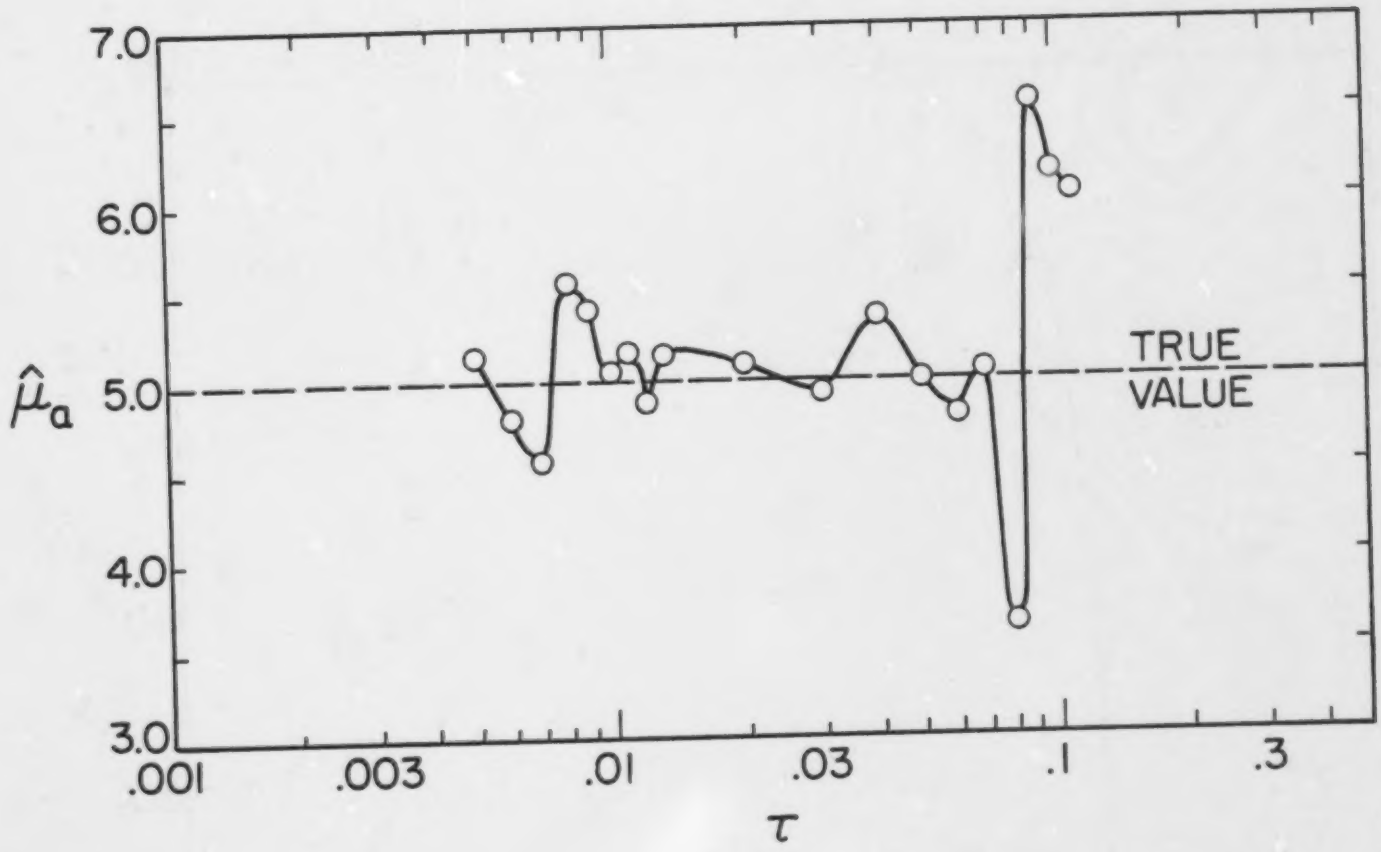


Figure 5. Spectral graph of the estimated mean value for a_{12} of Smith's model.

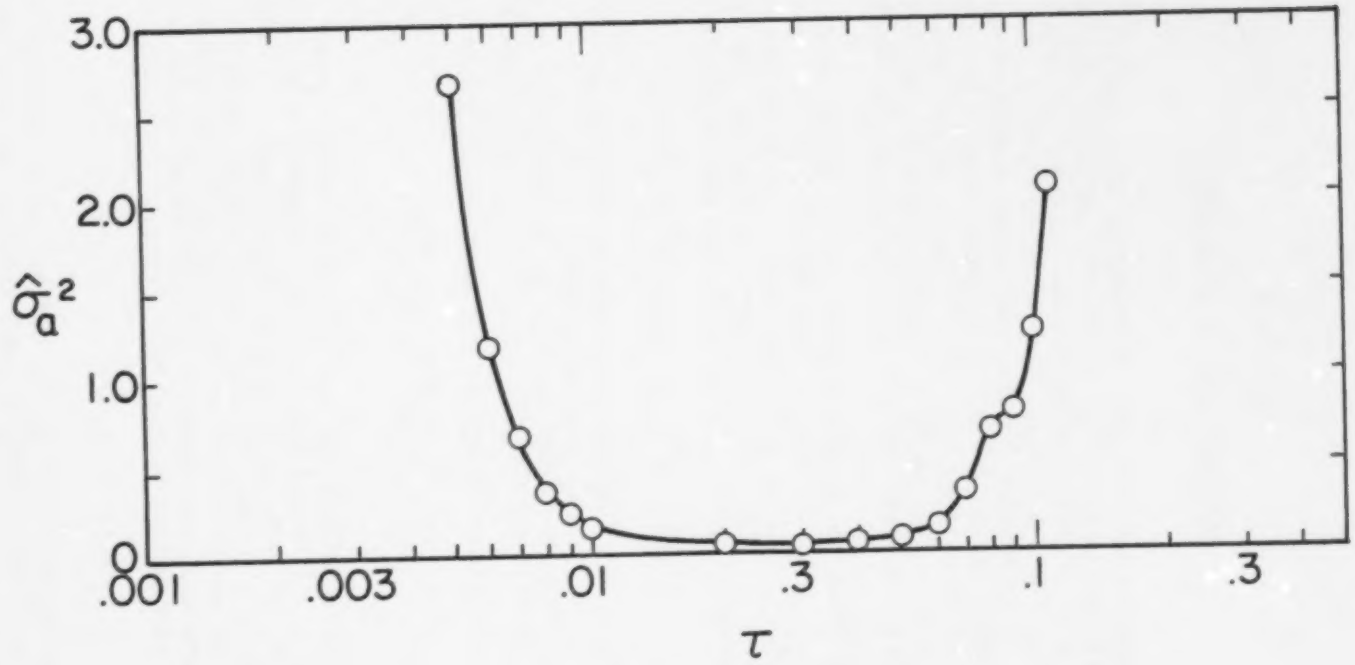


Figure 6. Spectral graph of the estimated variance for a_{12} of Smith's model.

SECTION 4

FREQUENCY DOMAIN TECHNIQUES

For both ecosystem modeling and experimental data analysis, the techniques of frequency domain analysis, using the Fourier series and transform, are becoming more popular with ecologists, e.g., see Platt and Denman (1975), Waide et al. (1974), Shugart (1978), Emanuel et al. (1978), and Van Voris et al. (1978). This is intriguing because the common method of analysis for determining the sample period for a communication system involves the frequency domain concept of bandwidth, expressed in terms of the Nyquist theory. Therefore, it would be useful to have a system bandwidth defined for the sampling and quantizing precesses used in the solution of the identification problem.

A transfer function can be defined for linear systems with one input $u(t)$ and one output $x(t)$. When the single input equals the unit impulse, also called the Dirac delta function $\delta(t)$, the output is called the impulse response and is denoted by $h(t)$. The transfer function for the system is then defined as the Fourier integral transform of the impulse response:

$$H(f) = \int_{-\infty}^{\infty} h(t)\, e^{-i\omega t} dt \qquad (4.1)$$

where $H(f)$ is the transfer function, $f = \omega/2\pi$ is the frequency independent variable measured in reciprocal time units and $i = \sqrt{-1}$.

A sequence of n transfer functions for an ecosystem can be defined by choosing, in turn, each compartment x_j $(j = 1, \ldots, n)$ of the state vector $\underline{x}$ as an output. The n transfer functions are then calculated by using

$$H_j(f) = \int_{0}^{\infty} x_j(t) e^{-i\omega t} dt \qquad (4.2)$$

for all $j = 1, \ldots, n$.

Transfer functions reflect the dynamics of a system through the concept of bandwidth, loosely defined as the range of frequencies which the system described by $H(f)$ passes in a relatively unchanged form. Carlson (1975) notes that the rate at which a system can vary stored energy is determined by the frequency response to perturbations as measured by the bandwidth. Thus, for ecosystems, bandwidth and compartmental turnover appear to be related.

The so-called bandlimited systems have transfer functions which satisfy

$$H(f) = 0, \text{ for all } f > B. \qquad (4.3)$$

For such systems the bandwidth is easily defined to be equal to B. However, most systems, including ecosystems, are not bandlimited, so other methods of defining the bandwidth are employed. One such method, called by Carlson

(1975) the effective bandwidth, uses the equal area concept. Consider Figure 7 which plots and compares the amplitude of a typical transfer function (the solid curve) with that of a rectangular window (the dashed curve). The rectangular window is clearly bandlimited with bandwidth of B. The effective bandwidth for H(f) is equal to B under the constraint:

$$2B \mid H(0) \mid = \int_{-\infty}^{\infty} \mid H(f) \mid df \tag{4.4}$$

which amounts to finding B to give equal area under the two curves.

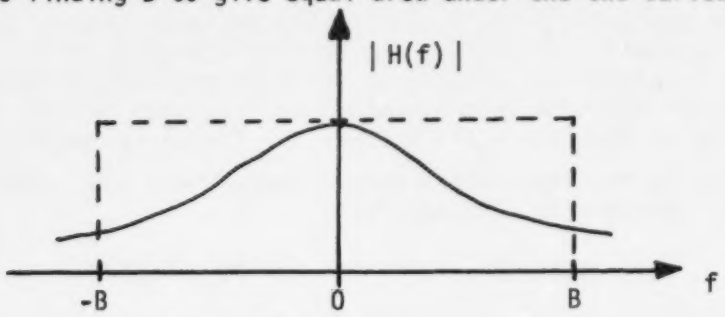


Figure 7. Effective bandwidth construction.

It is now possible to compute the bandwidth for the ecosystem transfer functions defined by (4.2). First, recall that $x_j(t)$ is amplitude limited by (3.2). Next, let f = 0 in (4.2), giving

$$H_j(0) = \int_{0}^{\infty} x_j(t)dt. \tag{4.5}$$

Substituting (3.2) into (4.5), gives the following inequality

$$1/\alpha \leq H_j(0) \leq 1/\delta \tag{4.6}$$

which holds for all j = 1, ... , n. In order to complete the computation of B from (4.4), it is necessary to evaluate the integral which appears in this equation. Estimating this integral is possible through the definition of the inverse Fourier transform:

$$x_j(t) = \int_{-\infty}^{\infty} H_j(f)e^{i\omega t}df. \tag{4.7}$$

Taking absolute values of (4.7) for all t > 0 and j = 1, ... , n, yields

$$1 \leq \int_{-\infty}^{\infty} \mid H_j(f) \mid df. \tag{4.8}$$

It is not possible to fully combine the inequalities (4.6) and (4.7) into (4.4) to estimate the bandwidth, the best result being $1 \leq 2B/\delta$. Thus, the bandwidth of an ecosystem depends upon turnover, but not in the ordinary sense. This result implies the bandwidth B to be greater than or equal to one-half the minimum exogenous turnover, that is the transfer rate of material out of the system to the environment.

For bandlimited frequency domain representations, the Nyquist sampling theorem gives $\tau_n \leq B/2$, where τ_n is the sample period from which measured data

can be used to reconstruct continuous time functions of system responses. The two inequalities derived are incommensurate, however assuming $\delta = 2B$ as a rule of thumb, the Nyquist result implies that ecosystems should be sampled with a sample period less than or equal to the reciprocal of the minimum exogenous turnover. Another rule of thumb is obtained by assuming equality in (4.8) and $H_j(0)\alpha = 1$ in (4.6) giving $2B/\alpha = 1$. Since $\alpha/2 = T_o^{-1}$, the bandwidth of an ecosystem is then equal to the maximum compartmental turnover.

For systems which are not bandlimited the bandwidth concept is at least elusive. The bandwidth of an ecosystem has not been clearly defined, therefore it may be useful to consider the results presented in the light of an example. As an elementary example of the frequency domain techniques presented, consider again Smith's hypothetical ecosystem defined by (3.16).

The transfer function $H_j(f)$ defines the frequency response of compartment j with respect to the input which enters compartment one. The Bode plot for the amplitude response is obtained from

$$\text{Logarithmic gain} = 20 \log_{10}|H_j(f)|, \qquad (4.9)$$

which is measured in units of decibels (db). Plots of (4.9) for the three compartmental transfer functions of Smith's model are given in Figure 8. These Bode plots of the system transfer functions, each of which contains several poles and zeros, are obtained by adding the individual plots due to each pole and zero. Furthermore, this procedure is simplified by using only the asymptotic approximations to these curves, as shown in Figure 8. These Bode plots describe the frequency response of the example ecosystem.

From (3.16) simple calculations yield $\delta = 2$ and $\alpha = 190$. Therefore, using $\tau = \sqrt{\tau^+\tau^-}$ and (3.6) and (3.4), the sample period is $\tau = 0.00078$ day for $d = 4$, which can be rounded to $\tau = 0.001$ day.

As for the ecosystem bandwidth, the inequality $1 \leq 2B/\delta$ gives $B \geq 1$(1/day). Figure 8 indicates the bandwidth to be approximately equal to 100 (1/day). Equating $\tau_n = \tau$, results in $B \leq 500$ (1/day). Thus, the inequality $1 \leq 2B/\delta$ yields very little useful information regarding the bandwidth of this ecosystem, but the rule of thumb, derived as $2B/\alpha = 1$, gives $B = 95$ (1/day) which seems reasonable.

Consider Figure 8 and measure the logarithmic gain at $f = 95$ (1/day) for each compartmental transfer function. Note that $|H_1(95)| > |H_2(95)| > |H_3(95)|$, which implies $B_1 > B_2 > B_3$ as an ordering of the bandwidths for the transfer functions of the three compartments. This ordering in turn implies $T_1 < T_2 < T_3$ for the three compartmental turnover times where $T_j = 1/a_{jj}$. The ordering of the turnover times given is ecologically reasonable. In this open (flow through) system, the phosphorus dynamics of the water compartment are fast, more rapid than the uptake and transfer of phosphorus by the plants. Also, the dynamics of phosphorus in the plants should be faster than for animals, as indicated. All this tends to add ecological intuition to the interpretation of the mathematics of determining the ecosystem bandwidth using $B = T_o^{-1}$.

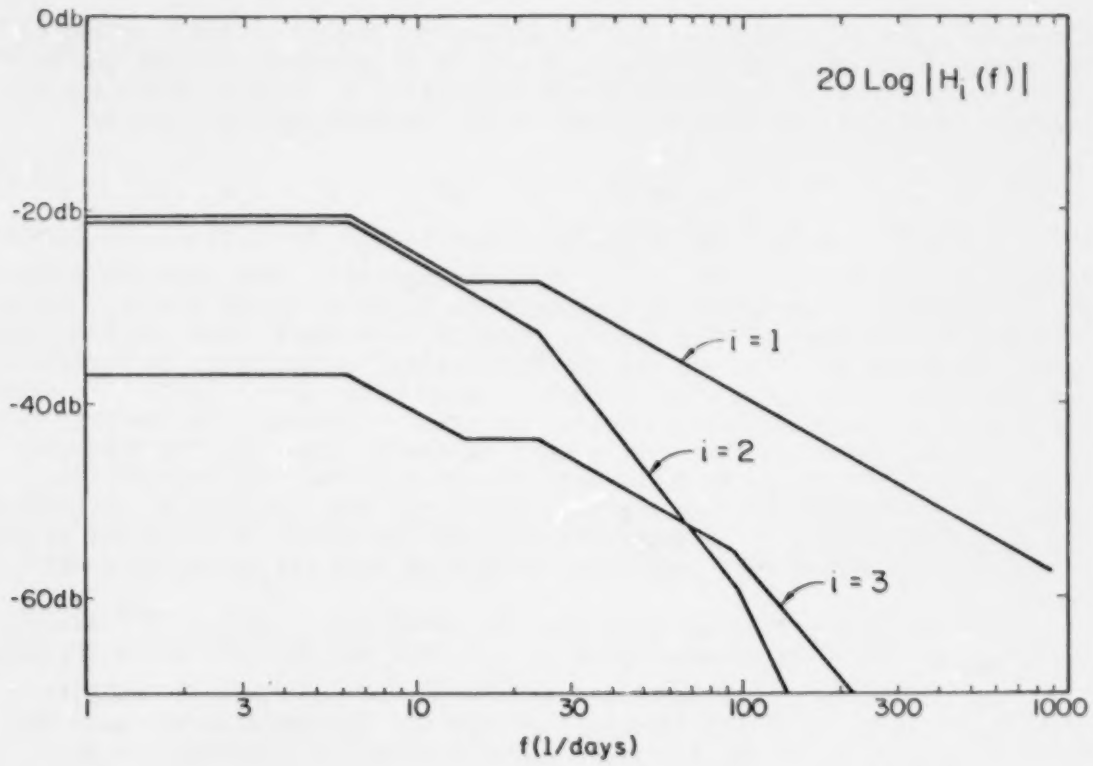


Figure 8. Example Bode plot.

For systems which are not bandlimited the frequency domain concept of bandwidth is inexact. Thus, the bandwidth of an ecosystem is not clearly defined. However, based upon the calculations presented in this paper, $B = T_o^{-1}$, taken as an approximation, appears to be useful in expressing the ecosystem bandwidth as the maximum compartmental turnover.

The Mulholland-Gowdy theory for the periodic sampling of ecosystem structure gives

$$\tau^- < \tau < \tau^+, \tag{4.10}$$

where the upper (τ^+) and lower (τ^-) bounds on the sample period τ depend on the system turnovers, the arithmetic precision of the data, and the number of system compartments. Processing of the transition state data, which are of bandpass character, requires a window in the frequency domain given by

$$f_\ell \leq f \leq f_u, \tag{4.11}$$

where $f_u = 1/\tau^-$ and $f_\ell = 1/\tau^+$ describe, respectively, the highest and lowest frequency (f) present in the data. If an assumption is made that the deterministic system is perturbed by a white noise Gaussian random process, which contains all frequencies with equally probable magnitudes, then the high frequency noise can be filtered from the experimental measurements by bandlimiting data plus noise to an upper frequency bound given by $f = 1/\tau^-$. Although the transition state data is bandpass, the steady-state data is low pass requiring measurements at essentially zero frequency, hence the low frequency noise cannot be filtered from the data as easily as the high frequencies. Least squares methods of data analysis remain the best solution to minimizing low frequency noise. It is important to study the effect of filtering on the error analysis of the data plus noise which come from the microcosm experiments.

For Smith's hypothetical ecosystem the value for τ^- is 5×10^{-4} assuming $\delta = 2$ and $d = 4$. This gives a value of $f_u = 2000$ per day, for which the Bode plots for all three compartments are well below -60 db. Thus, a low pass filter with an upper cutoff frequency of 2000 per day would surely pass the information content of the microcosm experiments while rejecting the high frequency noise present in the data.

SECTION 5

IDENTIFIABILITY

Before implementation of the identification algorithm, conditions should be investigated that will insure the uniqueness of a numerical estimation of the associated parameters. A *priori* knowledge of which and/or how many parameters of the flow matrix A can be determined by means of the chosen input-output experiment is termed identifiability (Cobelli, 1976). If the internal couplings cannot be uniquely determined, changes in the mathematical model structure or the experiment itself must be modified. Therefore, an identifiability analysis may be considered as a necesseary step preceding identification.

Often, identification is derived from numerical values of a few known parameters and is reduced to a problem of state estimation in which it is natural to deal with identifiability in a probabilistic manner. Identifiability in such stochastic systems may be defined by the existence of an estimator (Tse, 1973, 1978) or by the uniqueness of the probability distribution function (Bowden, 1973). A survey of similar investigations is provided by Reid (1977). In the study of biological systems, identification often depends upon *a priori* knowledge of the model structure (at least the order) and it is appropriate to use a deterministic canonical system approach to the determination of model parameters. Other approaches to the problem include parametrization (Glover, 1974) and parameter sensitivity analysis (Reid, 1977), which are both closely related to transfer function methods.

An explicit discussion of the problem of structural identfiability in the frequency domain is given by Bellman and Astrom (1970) where they propose the use of the transfer function to investigate identifiability. Consider the system

$$\dot{\underline{x}}(t) = \underline{A}\,\underline{x}(t) + \underline{B}\,\underline{u}(t) \tag{5.1a}$$

$$\underline{y}(t) = \underline{C}\,\underline{x}(t) \tag{5.1b}$$

which is the linear compartment model defined by (3.1) with a single dose input $\underline{u}(t)$, where $\underline{y}(t)$ is an m-vector of measurements of the state $\underline{x}$ and $\underline{C}$ is a p x n connectivity matrix of the form

$$C_{ij} = \begin{cases} 1 \\ 0 \end{cases} \tag{5.2}$$

and

$$\sum_{j=1}^{n} C_{ij} = 1$$

for all i = 1, ... , p. Let $\underline{Y}(s)$ be the Laplace transform of $\underline{y}(t)$ and $\underline{U}(s)$ that of $\underline{u}(t)$. Then

$$\underline{Y}(s) = \underline{G}(s)\,\underline{U}(s) \tag{5.3}$$

where $\underline{G}(s)$ is the transfer matrix given by

$$\underline{G}(s) = \underline{C}(s\underline{I} - \underline{A})^{-1}\,\underline{B} \tag{5.4}$$

and $\underline{I}$ is the n-th order identity matrix. The problem of identifying the flow matrix $\underline{A}$ from the experimental data may be reduced to that of identifying the coefficients of the transfer matrix, each coefficient being a combination of the elements of $\underline{A}$. Therefore, the $\underline{A}$ matrix is identifiable when this non-linear system of equations has a unique solution.

Lin and Yu (1977) considered the single input and single output special case of (5.1) in canonical form, where $\underline{A}$ is the companion matrix associated with the characteristic polynomial

$$s^m + a_{m-1}\,s^{m-1} + \ldots + a_1 s + a_0 = 0 \tag{5.5}$$

and

$$\underline{C} = [c_1 c_2 \ldots c_n] \tag{5.6}$$

$$\underline{B}^T = [\,0\ 0 \ldots 1]. \tag{5.7}$$

This leads to a scalar input/outout formulation for (5.3) in which G(s) contains 2n unknown parameters (n poles, n-1 zeros, and a gain factor). The identification of these parameters is demonstrated by a time series analysis of the output variable given by

$$y(t) = \gamma_1 e^{\lambda_1 t} + \ldots \gamma_n e^{\lambda_n t}.$$

A numerical algorithm called Prony's method (Hildebrand, 1974) is applied to y(t) in order to resolve the parameters λ_i and γ_i of the exponential curve fit. The λ_i and γ_i parameters are then shown to uniquely determine the 2n unknown parameters of $\underline{G}(s)$.

The precise definition of identifiability provided by Bellman and Astrom (1970) is equivalent to saying that the parameters of $\underline{A}$ are identifiable if and only if any change in the values of the coefficients causes a change in the measured quantities $\underline{y}(t)$. Thus, a necessary condition for identifiability is that a system be controllable and observable in the sense of Kalman (1963).

Definition 5.1

A linear system is said to be completely state controllable if for any initial state at t_o it can be driven to any other state in the state space at t = T.

Definition 5.2

A linear system is said to be completely output controllable if it is possible to drive any initial output at t_0 to any final output in a finite time interval.

Definition 5.3

A linear system is said to be completely observable if for every initial time t_0 and some finite time T_1, $t_0 \leq t \leq T_1$ every initial state at t_0 can be determined from the knowledge of the output on $t_0 \leq t \leq T$.

Rigorous treatments on the properties of controllability and observability can be found in system theory literature (Kalman, 1963; Luenberger, 1963; Lee, 1964; Ogata, 1967; and Chen, 1970). In the following, these properties will be considered as they apply to the previously discussed methods of identification for compartmental models.

DIRECT METHOD

Assume that a single dose of tracer may be directly inserted via special routes into system compartments and that tracer behavior can be experimentally monitored in specified compartments when the system is switched to a tracer-free environment. The controllability and observability of such a system has been explicitly discussed by Bellman and Astrom (1970) and Johnson (1976).

A system described by (5.1) is controllable if and only if the column vectors of the n x nm test matrix

$$\underline{P}_c = [\underline{B}; \underline{AB}; \underline{A}^2\underline{B}; \ldots; \underline{A}^{n-1}\underline{B}] \tag{5.8}$$

span the n-dimensional space on which $\underline{x}(t)$ is defined. In other words, $\underline{P}_c$ must be of rank n if the system is to be controllable (Kalman, 1963).

Definition 5.4

A system is open (closed) when there is some (no) exchange of material from the system either to the environment or to another subsystem. Using the properties of the controllability matrix $\underline{P}_c$, Johnson (1976) shows that closed systems are uncontrollable regardless of their structure. Open systems are also examined and are found to be controllable, in general, if the flow matrix $\underline{A}$ is of rank n or (n-1) and at least one flow between the system and its environment is controlled. Necessary conditions for complete controllability can also be derived from physical reasoning. Cobelli and Romanin-Jacur (1976) adopt a structural point of view by relating controllability and observability of compartmental systems to their experimental design. A system is shown to be completely controllable only if there exists at least one path from some input to every compartment. In addition, it should be noted that the specification of bounds on the controlled elements implies that a system otherwise completely controllable must now have a restricted range of controllability in state space.

The concept of observability of a dynamic system is associated with the processing of data obtained from measurements on the system. Analogous to the

test for controllability, Kalman (1963) has shown that a linear, time-invariant system defined by (5.1) is observable if and only if the n x np matrix

$$\underline{P}_o = [\underline{C}^T; \underline{A}^T\underline{C}^T; (\underline{A}^T)^2\,\underline{C}^T; \ldots; (\underline{A}^T)^{n-1}\underline{C}^T] \qquad (5.9)$$

is of rank n. If there is only one output (p = 1) then a necessary and sufficient condition for observability is that $\underline{P}_o$ be nonsingular. The test for observability may be applied to compartmental models by utilizing techniques that were employed when discussing controllability. Upon inspection of the definition of observability, it is clear that observability does not depend upon the controlled input matrix, but rather on the output matrix. A linear compartment model, in the structural sense, is completely observable if at least one output is reachable from every compartment. It is also necessary that no outputs be associated with only the state components which form one or more sink, all influencing the same outputs (Cobelli and Romanin-Jacur, 1976).

Definition 5.5

A subsystem of compartments which receives input from the remainder of the system, but has no transfers out of the subsystem from any of its compartments, is called a trap. A trap may also be called a closed subsystem.

It is important to mention that the conditions given for controllability and observability are not sufficient, that is, the preceding conditions neither guarantee the identifiability of $\underline{A}$, nor are the elements of $\underline{A}$ in the uncontrollable and unobservable part of the system necessarily unidentifiable. Counter-examples which clarify these points are considered by Distefano (1977). Bellman and Astrom (1970) emphasize the difficulty of the problem of identifiability and since that time, only necessary conditions have been related in the literature. Cobelli and Romanin-Jacur (1976) give criteria for sufficient conditions, but a close study (Delforge, 1977) shows by counter-example that the proposed criteria are necessary, but not sufficient. The problem reduces to a recurring mathematical question which asks how many solutions a set of nonlinear equations has.

Let $\underline{A}$ be unidentifiable. Then it may be possible to formulate an experiment to show that a subset of compartmental levels can be controllable even when the system fails to meet controllability and observability requirements (Johnson, 1976). For example, consider a system in which certain states are, for biological reasons, not accessable and their evaluation, according to the structural identifiability tests, is not possible. If a feasible experimental condition can be obtained by adding a new input, thereby yielding necessary conditions, the system may be considered identifiable (Milanese, 1976). Also, it has been suggested that the simplest way to deal with a multicompartment system is to ignore closed subsystems if possible because any or all of the traps can be deleted without altering the behavior of the rest of the system (Thron, 1972). In general, this is possible with regard to measurements on compartments of completely open subsystems; and most systems utilizing the direct method for identification of the $\underline{A}$ matrix would fall into this category. However, certain observations, such as the kinetics of urinary excretion, require the use of an indirect measurement and hence the accumulation pools may not be excluded. Necessary conditions for identifiability are therefore derived for the indirect algorithm.

INDIRECT METHOD

The necessary conditions given for controllability and observability of a system for the direct identification algorithm imply that any model of a real system with one or more compartments acting as stores for the system may not be identifiable. With the indirect scheme, the observer states $\underline{y}$ form a set of flows disjoint from the internal couplings, each accumulation compartment being a singular trap. In this section, criteria are investigated for controllability and observability related to compartmental structure of a system having ℓ accumulation pools ($\ell \leq n$) from which all observations are to be made. The local model of (3.1) is again incorporated along with the linear differential observer for the accumulation pools:

$$\dot{\underline{y}} = \underline{K}\,\underline{x} \tag{5.10a}$$

which can be combined to give

$$\begin{bmatrix} \dot{\underline{x}} \\ \dot{\underline{y}} \end{bmatrix} = \begin{bmatrix} \underline{A} & \underline{0} \\ \underline{K} & \underline{0} \end{bmatrix} \begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix} + \begin{bmatrix} \underline{B} \\ \underline{0} \end{bmatrix} \underline{u} \tag{5.10b}$$

from which the total system behavior may be explored. Now define the measurement vector $\underline{z}$ as follows:

$$\underline{z} = [\underline{0} \quad \underline{I}] \begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix}. \tag{5.10c}$$

Measurements are to be taken from each of the n observer states. The system described by (5.10) is controllable if and only if the partitioned matrix

$$\underline{P}_{ic} = \begin{bmatrix} \underline{P}_1 \\ \underline{P}_2 \end{bmatrix} = \left[\begin{bmatrix} \underline{B} \\ \underline{0} \end{bmatrix} \begin{bmatrix} \underline{AB} \\ \underline{KB} \end{bmatrix} \begin{bmatrix} \underline{A^2B} \\ \underline{KAB} \end{bmatrix} \begin{bmatrix} \underline{A^3B} \\ \underline{KA^2B} \end{bmatrix} \cdots \begin{bmatrix} \underline{A^{n-1}B} \\ \underline{KA^{n-2}B} \end{bmatrix} \right] \tag{5.11}$$

spans the $(\ell + n)$ state space on which the system is defined, where the two $n \times nm$ submatrices $\underline{P}_1$ and $\underline{P}_2$ are called the upper and lower partitions, respectively, of the controllability matrix. Now if $\underline{P}_{ic}$ is of rank $2n$, then $\underline{P}_1$ and $\underline{P}_2$ must both be of full rank. Note that the upper partition of the controllability matrix is the same test matrix as that for the direct method (see equation (5.8)). Thus, as with the direct method, if there is no path from any input to compartment i, then the i-th row of the controllability matrix is identically null, as no input enters compartment i. Next consider the lower partition of the matrix $\underline{P}_{ic}$. If, in addition to the aforementioned condition, there is no accumulation compartment that can be reached from a given compartment i, then every element of the i-th row of the controllability matrix is

null as no pool is influenced by the state variable associated with the i-th compartment.

For a clearer understanding of the observer portion of the controllability matrix, consider the dynamic states $\underline{y}$ to be continuous observations rather than accumulation pools. Then from Kalman (1963) and the definition of output controllability, the system is said to be completely output controllable if and only if the composite matrix

$$\underline{P}_{oc} = [\underline{KB};\ \underline{KAB};\ \underline{KA}^2\underline{B};\ \ldots;\ \underline{KA}^{n-1}\underline{B};\ \underline{D}] \tag{5.12}$$

is of the same rank as the row order of $\underline{K}$, where $\underline{D}$ is the connectivity matrix which postulates a direct transmission from $\underline{u}$ to $\underline{y}$. The existence of a direct input into any accumulation pool is not assumed to exist, that is, $\underline{D} = \underline{0}$. In fact, if the same compartment is available for insertion and observation of tracer, identification requires that the associated flow matrix be irreducible (Smith, 1976), whereas the flow matrix for the indirect identification scheme is reducible. Thus, tracer must be injected into the internal system $\underline{x}$ and not into the observer $\underline{y}$. If the rank of the ℓ x nm matrix

$$\underline{P}_2 = [\underline{0};\ \underline{KB};\ \underline{KAB};\ \underline{KA}^2\underline{B};\ \ldots;\ \underline{KA}^{n-2}\underline{B}] \tag{5.13}$$

is of rank ℓ, then the rank of the ℓ x nm matrix $\underline{P}_{oc}$ given by (5.12) is necessarily ℓ. Notice that state controllability is neither necessary nor sufficient for output controllability.

The discussion of indirect controllability to this point has relied upon the knowledge of the rank of $\underline{P}_{ic}$ which is not customarily known when discussing identifiability. Conditions must be placed upon the submatrices $\underline{P}_1$ and $\underline{P}_2$ such that the indirect controllability matrix will be of rank $\ell + n$, giving a necessary condition for identifiability.

Definition 5.6

A system is said to be reduced controllable if and only if the rank of the matrix $\underline{P}_k$ where

$$\underline{P}_k = [\underline{B};\ \underline{AB};\ \underline{A}^2\underline{B};\ \ldots;\ \underline{A}^{k-1}\underline{B}] \tag{5.14}$$

is n. The smallest possible integer k for which $\underline{P}_k$ is of rank n will be called the reduced order. Sufficient conditions for the controllability matrix $\underline{P}_{ic}$ to be of the desired rank follow.

Definition 5.7

Two m x n matrices are defined to be equivalent if and only if one may be transformed into the other by nonsingluar elementary row and column transformations. If $\underline{A}$ and $\underline{B}$ are equivalent, we write

$$\underline{A} \overset{E}{=} \underline{B} \tag{5.15}$$

Theorem 5.1

A system given by (5.1) in which measurements are obtained from ℓ accumulation pools is controllable if the test matrix $\underline{P}_{ic}$ (5.11) of the system is such that

(i) The upper partition $\underline{P}_1$ is a reduced controllability matrix $\underline{P}_k$ with $2k < n-1$, where n is the rank of $\underline{A}$ and k is the reduced order of the controllability matrix, and

(ii) $\underline{CA}^k\underline{P}_k$ is of rank ℓ.

Proof:

Rewrite the indirect controllability matrix as

$$\underline{P}_{ic} = \begin{bmatrix} \underline{P}_1 \\ \underline{P}_2 \end{bmatrix} = \begin{bmatrix} \underline{B}; \underline{AB}; \ldots; \underline{A}^k\underline{B}; & \underline{A}^{k+1}\underline{B}; \ldots; \underline{A}^{n-1}\underline{B} \\ \underline{0}; \underline{KB}; \ldots; \underline{KA}^{k-1}\underline{B}; \underline{KA}^k\underline{B}; \ldots; & \underline{KA}^{n-2}\underline{B} \end{bmatrix} \tag{5.16}$$

Now if the matrix $\underline{P}_1$ is reduced controllable, then $\underline{P}_k$ is of rank n where

$$\underline{P}_k = [\underline{B}; \underline{AB}; \ldots; \underline{A}^k\underline{B}]. \tag{5.17}$$

Since $\underline{P}_k$ is of rank n, then $\underline{P}_1$ is of rank n and

$$\underline{P}_1 \overset{E}{=} [\underline{I}; \underline{0}] \tag{5.18}$$

where $\underline{I}$ is the n-th order identity matrix. Next multiply the matrix $\underline{P}_1$ by $\underline{CA}^k$, yielding

$$\underline{P}'_k = [\underline{CA}^k\underline{B}; \underline{CA}^{k+1}\underline{B}; \ldots; \underline{CA}^{2k}\underline{B}]. \tag{5.19}$$

If $2k < n-1$, then $2k$ is at most $n-2$ so that if $\underline{P}'_k$ is of rank ℓ, then

$$\underline{P}''_k = [\underline{CA}^k\underline{B}; \underline{CA}^{k+1}\underline{B}; \ldots; \underline{CA}^{n-2}\underline{B}] \tag{5.20}$$

is of rank ℓ. (Recall that the rank of a product is less than or equal to the rank of either matrix. Therefore, the matrix $\underline{C}$ is at most of rank ℓ.) Notice that $\underline{P}_2$ can be rewritten as

$$\underline{P}_2 = [\underline{0}; \underline{CB}; \ldots; \underline{CA}^{k-1}\underline{B}; \ldots; \underline{P}''_k] \tag{5.21}$$

and if $\underline{P}'_k$ is of rank n, then

$$\underline{P}_2 \overset{E}{=} [\underline{0}; \underline{I}'] \tag{5.22}$$

where $\underline{I}'$ is the ℓ-th order identity matrix. Therefore

$$\underline{P}_{ic} = \begin{bmatrix} \underline{P}_1 \\ \underline{P}_2 \end{bmatrix} \overset{E}{=} \begin{bmatrix} \underline{I} & \underline{0} \\ \underline{0} & \underline{I}' \end{bmatrix} = \underline{I}'' \tag{5.23}$$

where $\underline{I}''$ is an $(n+\ell) \times (n+\ell)$ identity matrix. Thus, the indirect controllability matrix $\underline{P}_{ic}$ is of rank $(n+\ell)$ which is a necessary and sufficient condition for controllability.

Two special cases of the indirect controllability matrix are to be investigated.

Case 1. If $\underline{B}$ and $\underline{CB}$ are nonsingular, then the matrix $\underline{P}_{ic}$ is of rank $\ell + n$. This result follows because $\underline{P}_{ic}$ can be regularly partitioned into a triangular block matrix

$$\underline{P}_{ic} \triangleq \begin{bmatrix} \underline{B} & \underline{0} \\ \underline{0} & \underline{CB} \end{bmatrix} \tag{5.24}$$

which is nonsingular if and only if each diagonal box is nonsingluar (Parker and Eaves, 1960).

Case 2. If $\underline{C}$ is the $n \times n$ accumulative flow matrix of (5.1) which is used in the indirect algorithm, $\underline{C}$ is nonsingular because all flows are on the diagonal. Now if the matrix $\underline{A}$ is multiplied on either side by a nonsingular matrix, the product has the same rank of $\underline{A}$. That is, the rank of $\underline{CA}$ is n. It follows that the rank of $\underline{CA}^k$ is n and if $\underline{P}_k$ is of rank n, then $\underline{CA}^k\underline{P}_k$ is of rank n. In theorem (5.1), the matrix $\underline{CA}^k\ \underline{P}_k$ had to be of the rank $\underline{C}$. Therefore, in the special case where there is an accumulation pool for each compartment, this condition is automatically satisfied.

Theorem 5.2

For indirect identification, there must be at least two inputs to the compartmental system.

Proof:

The number of accumulation pools within a system is assumed to be less than or equal to the number of compartments in the system. That is, $\ell \leq n$. In addition, the number of rows in $\underline{P}_{ic}$ must be at most equal to the number of compartments n times the number of inputs m, or

$$\ell + n \leq nm. \tag{5.25}$$

Now divide both sides of (5.25) by n, yielding

$$\frac{\ell}{n} + 1 \leq m, \tag{5.26}$$

but since $\ell \leq n$, then $\frac{\ell}{n} \leq 1$ and unless $\ell = 0$ (which is the direct method), $m \leq 2$ because there can be no partial inputs.

Measurements of the accumulation pools are to be obtained for identification of the system of equations (5.10). In order for the system to be able in the sense of Kalman (1963), it is necessary and sufficient that the

test matrix

$$\underline{P}_{io} = \begin{bmatrix} \underline{P}_3 \\ \underline{P}_4 \end{bmatrix} = \begin{bmatrix} \underline{0}; \ \underline{K}^T; \ \underline{A}^T\underline{K}^T; \ \ldots; \ \underline{A}^{T^{n-2}}\underline{K}^T \\ \underline{I}'; \ \underline{0}; \ \underline{0}; \quad \ldots; \ \underline{0} \end{bmatrix} \tag{5.27}$$

is of rank n + ℓ where $\underline{I}'$ is the ℓ-th order identity matrix. Note that if the submatrix $\underline{P}_3$ is of rank n, then

$$\underline{P}_3 \overset{E}{=} [\underline{0}; \ \underline{I}] \tag{5.28}$$

where $\underline{I}$ is the n-th order identity matrix and hence,

$$\underline{P}_{io} = \begin{bmatrix} \underline{P}_3 \\ \underline{P}_4 \end{bmatrix} \overset{E}{=} \begin{bmatrix} \underline{0} & \underline{I} \\ \underline{I}' & \underline{0} \end{bmatrix} \overset{E}{=} \begin{bmatrix} \underline{I} & \underline{0} \\ \underline{0} & \underline{I}' \end{bmatrix} \tag{5.29}$$

giving an equivalent (n+ℓ) x (n+ℓ) identity matrix. Thus, for $\underline{P}_{io}$ to be of the desired rank, $\underline{P}_3$ must be of rank n. By considering the states $\underline{y}$ as continuous observations of the internal states $\underline{x}$, the necessary conditions presented by Cobelli and Romanin-Jacur (1976) for observability for the direct algorithm may be applied to the indirect scheme. In the structural sense, the indirect model is completely observable if at least one flow to an accumulation compartment is reachable from every internal compartment. In addition, no accumulative flows may be associated with only the internal state variables which form one or more traps, all influencing the same pool.

COMBINED DIRECT-INDIRECT

Applications of the direct and indirect algorithms may tend to overlap in certain systems. An introduced (labeled) substance may metabolize and accumulate, along with its metabolites, in one or more pools and also be directly measureable as an output from compartments within the system itself. In other systems, the outputs available for data collection might be the sum of observations from a compartment and its accumulation pool.

The method in which the observations are made is not involved in controllability which is concerned with the flow of the inputs, so the indirect controllability conditions suffice for the combined measurement technique.

Observability of the two types of combined systems will be discussed in this section. Requirements for observability are straightforward. First consider the system of (5.10) where the measurement vector is of the form

$$\underline{z} = \begin{bmatrix} \underline{C} & \underline{0} \\ \underline{0} & \underline{I} \end{bmatrix} \begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix}. \tag{5.30}$$

Measurements are to be collected from both system compartments and accumulation pools. The system is observable if and only if the test matrix

$$\underline{P}_{di} = \left[\begin{array}{c:ccc:ccc} \underline{0}; \underline{C}^T & \underline{A}^T\underline{C}^T; & \ldots; & (\underline{A}^T)^{n-1}\underline{C}^T & \underline{0}; \underline{K}^T; & \underline{A}^T\underline{K}^T; & \ldots; & (\underline{A}^T)^{n-2}\underline{K}^T \\ \underline{I} & & \underline{0} & & & \underline{0} & & \end{array}\right] \quad (5.31)$$

is of the rank p + ℓ where $\underline{I}$ is an ℓ-th order identity matrix. Define the upper partition to be

$$\underline{P}'_{di} = [\underline{0}; \ \underline{P}_5; \ \underline{P}_6] \quad (5.32)$$

and notice that $\underline{P}_5$ is the observability matrix $\underline{P}_o$ for the direct algorithm while $\underline{P}_6$ is the observability matrix $\underline{P}_{io}$ for the indirect scheme for identification. The system is completely observable if the conditions for direct observability are satisfied because $\underline{P}_5$ would be of rank p, making the system

$$\underline{P}_{di} \overset{E}{=} \begin{bmatrix} \underline{I}' & \underline{0} & \underline{P}_6 \\ \underline{0} & \underline{I} & \underline{0} \end{bmatrix} \quad (5.33)$$

of rank p where $\underline{I}'$ and $\underline{I}$ are p-th order and ℓ-th order identity matrices, respectively. Also, if there are as many (or more) accumulation pools as directly measureable states (p), and the conditions for indirect observability hold, then the system is of the form

$$\underline{P}_{di} = \begin{bmatrix} \underline{I}' & \underline{0} & \underline{P}_5 \\ \underline{0} & \underline{I} & \underline{0} \end{bmatrix} \quad (5.34)$$

and the desired rank is obtained. In addition, if the two test matrices (direct and indirect) combine to form a matrix $\underline{P}_7$ of rank p, the system becomes

$$\underline{P}_{di} = \begin{bmatrix} \underline{0} & \underline{P}_7 \\ \underline{I} & \underline{0} \end{bmatrix} \overset{E}{=} \begin{bmatrix} \underline{I}' & \underline{0} \\ \underline{0} & \underline{I} \end{bmatrix} \quad (5.35)$$

and the necessary and sufficient conditions for identifiability are fulfilled.

Consider next a system which has as its output the sum of observations. In this combined case, the measurement vector for the system is

$$\underline{z} = [\underline{C} \quad \underline{I}] \begin{bmatrix} \underline{x} \\ \underline{y} \end{bmatrix} \quad (5.36)$$

and the system is said to be observable in the sense of Kalman (1963) if and only if the test matrix

$$\underline{P}_s = [\underline{C}^T; \ \underline{A}^T\underline{C}^T; \ \ldots; \ (\underline{A}^T)^{n-1}\underline{C}^T] + [\underline{0}; \ \underline{K}^T; \ \underline{A}^T\underline{K}^T; \ \ldots; \ (\underline{A}^T)^{n-2}\underline{K}^T] \quad (5.37)$$

is of rank p. Thus, the system is observable if the sum of the observability matrices for the direct and indirect algorithms is of rank p. However, two

matrices of different orders cannot be added, so in order for the test matrix $\underline{P}_s$ to be defined, the number of direct observations, p, must equal the number of accumulation pools, ℓ.

SECTION 6

CONSTANT INFUSION

A constant infusion input has occasionally been used in tracer methods to label compartments to a high specific activity. The constant influx of tracer was probably first incorporated by Hevesey and Hahn (1940) to obtain high concentrations of ^{32}P-phosphate in plasma. Hevesey and Hahn, however, were not interested in analyzing the data to determine model parameters. Constant infusion is also used when there are problems with incomplete and non-instantaneous mixing within compartments, usually due to spatial homogeneities. Shipley and Clark (1972) present textbook cases in which the method and its usage are discussed. Assuming that the chronic infusion of tracer does not disturb the behavior of the recipient compartments, then the constant input level of Table 1 gives rise to a steady-state defined by $\underline{x}_s$.

The constant infusion method as discussed in Section 3 is based upon the compartment model defined by (3.1) as

$$\dot{\underline{x}} = \underline{A}\underline{x} + \underline{B}\underline{u}. \tag{6.1}$$

Linearly independent inputs generate an ensemble of linearly independent steady-state samples of the system state $\underline{x}$ from which the coefficients of the matrix of rate coefficients may be determined.

When in steady-state, the system of (6.1) can be described by

$$\underline{0} = \underline{A}\underline{x} + \underline{B}\underline{u}. \tag{6.2}$$

Recall that $\underline{x}$ is an n-vector of compartmental states, $\underline{u}$ is an m-vector of specified inputs, and $\underline{B}$ is an n x m matrix where

$$b_{ij} = \begin{cases} 1 \\ 0 \end{cases}$$

$$\text{and} \quad \sum_{i=1}^{n} b_{ij} = 1.$$

Let $\underline{u}_1, \underline{u}_2, \ldots, \underline{u}_m$ span R^m. Assuming that the compartmental system is open so that $\underline{A}^{-1}$ exists, then $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_m$ span at most an m-dimensional subspace of R^n where

$$\underline{A}\,\underline{x}_k = -\underline{B}\,\underline{u}_k \qquad k=1, \ldots, m. \tag{6.3}$$

Now set

$$-\underline{B}\underline{u}_k = \underline{w}_k \qquad k=1, \ldots, m \tag{6.4}$$

which results in

$$\underline{A}\,\underline{X} = \underline{W} \tag{6.5}$$

where the n x m matrices

$$\underline{X} = [\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_m] \tag{6.6}$$

and

$$\underline{W} = [\underline{w}_1, \underline{w}_2, \ldots, \underline{w}_m] \tag{6.7}$$

are both of rank m. Taking the transpose of each side of equation (6.5) gives

$$\underline{X}^T \underline{A}^T = \underline{W}^T. \tag{6.8}$$

Next define the n-vector a_k to be the k-th column of $\underline{A}^T$ such that

$$\underline{A}^T = [\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_n] \tag{6.9}$$

The vectors $\underline{a}_k$ define the unknown system parameters, i.e., the rate coefficients of the compartment model. Thus,

$$\underline{X}^T \underline{a}_k = \underline{z}_k \qquad k=1, \ldots, n \tag{6.10}$$

where $\underline{z}_k$ is the m-vector of the k-th column of

$$\underline{Z} = \underline{W}^T \tag{6.11}$$

where

$$\underline{Z} = [\underline{z}_1, \underline{z}_2, \ldots, \underline{z}_n] \tag{6.12}$$

and rank ($\underline{Z}$) = m. It should be noted that the vectors $\underline{a}_k$ and $\underline{z}_k$ of (6.10) are completely determined by the compartmental inputs. That is, $\underline{a}_k$ represents the k-th row of $\underline{A}$ giving the endogenous inputs to the compartment and $\underline{z}_k$ defines the possibility of an exogenous input to compartment k.

Identifiability related to the system structure for a multi-input/multi-output system where all states can be measured directly is to be considered first. The system is structurally identifiable when the number of parameters that can be estimated is not smaller than the number of known system parameters in the algebraic equation (6.5).

Only compartment models which are open to their environment are considered in this chapter because closed systems with constant rate inputs accumulate material at a constant rate, never reaching steady-state. This condition does not prohibit the closure of an individual compartment or groups of com-

partments as long as they do not form a decoupled subsystem. The $\underline{A}$-matrix for an open system is characterized by a nonzero determinant. This result implies that in the special case when the inputs $\underline{u}_k$ (k=1, ..., n) span R^n, the resultant steady-states $\underline{x}_k$ (k=1, ..., n) also span R^n and $\underline{X}^{-1}$ exists. Hence, the matrix equation (6.5) can be solved by multiplying on the right by $\underline{X}^{-1}$, giving $\underline{A} = \underline{W}\underline{X}^{-1}$. Input access to every compartment in the system and the ability to measure all compartmental steady-states then imply structural identifiability. These sufficient conditions are only rarely met in practice, requiring for biochemical systems the organic synthesis of tracer material for all chemical species present in the system. For ecological systems, only a few natural input pathways to the system exist with many compartments being essentially inaccessable. Therefore, the remainder of this chapter concerns the development of conditions which relate identifiability to system structure with restricted compartmental access.

Theorem 6.1

A compartmental system is identifiable only if there exists at least one path from some constant input to every compartment.

Proof:

By contradiction, if there is no path from any input to one or more compartments, then for all k, equation (6.3) can be partitioned as

$$\begin{bmatrix} \underline{A}_1 & \underline{A}_2 \\ \underline{0} & \underline{A}_3 \end{bmatrix} \begin{bmatrix} \underline{x}_{k1} \\ \underline{x}_{k2} \end{bmatrix} = \begin{bmatrix} \underline{w}_k \\ \underline{0} \end{bmatrix} \tag{6.13}$$

Hence, the following relationships arise:

$$\underline{A}_1 \underline{x}_{k1} + \underline{A}_2 \underline{x}_{k2} = \underline{w}_k \tag{6.14}$$

But $\underline{A}_3^{-1}$ exists, that is, there are no closed subsystems, and the vector $\underline{x}_{k2}$ is identically null. Thus, regardless of the values of the elements comprising $\underline{A}_3$, the model parameters contained in $\underline{A}_3$ and $\underline{A}_2$ cannot be identified by solving equations of the form (6.10). Thus, structural identifiability depends on the ability of inputs to reach every compartment.

Theorem 6.2

A system is identifiable by the constant infusion method only if at least one outlet to the environment is reachable from every compartment along any path.

Proof:

By contradiction, if no system outlets can be reached from compartment m, then this compartment and all compartments coupled to it continuously accumulate material without reaching a steady-state. This, of course, prohibits identification using (6.5).

The preceding concepts of structural identifiability based upon the data derived from constant infusion experiments parallel those already known for the single dose method (see Section 5). However, the solution of the identification problem of a constant input applied to a system is further constrained by the static nature of the resultant steady-state. Indeed, as will be shown, the dynamic systems concept of observability plays no role in solving this algebraic problem.

Theorem 6.3

For m exogenous inputs $\underline{u}$ to an identifiable compartmental system, there can be at most (m-1) endogenous inputs to any single compartment k.

Proof:

For m inputs into a system, equation (6.10) produces m independent equations in the n unknown parameters of $\underline{a}_k$. But at most m unknowns can be determined from the solution of m independent equations. Recall that the k-th entry in the n-vector $\underline{a}_k$ represents the turnover of the k-th compartment. If the compartment turnover is to be estimated, then at most m-1 of the endogenous inputs to the k-th compartment (the remaining entries in $\underline{a}_k$) can be identified. Thus, for m inputs to a system, there can be at most m-1 endogenous inputs to a single compartment.

The (n-m) compartments r without exogenous inputs produce m dependent equations of the form

$$\underline{X}^T \underline{a}_r = \underline{0} \tag{6.16}$$

where $\underline{a}_r$ is defined as in equation (6.10). Therefore, (n-m) additional equations are needed for the solution of (6.5). The necessary equations may be obtained from each of the (n-m) compartments $\underline{a}_r$ in one of the following ways:

1. Turnover of x_r must be known from an independent measurement, or from *a priori* knowldege of the compartmental turnover, giving the r-th entry in $\underline{a}_r$.
2. Flow out of the compartment to the environment must be determined for an open compartment.
3. A closed compartment offers an additional independent equation given by the null column sum

$$\sum_{i=1}^{n} a_{ir} = 0 \tag{6.17}$$

where a_{ir} (i=1, ..., n) define the components of $\underline{a}_r$.

Consider the three compartment system of Figure 9 which gives an $\underline{A}$-matrix of unknown system parameters of the form

$$\underline{A} = \begin{bmatrix} a_{11} & 0 & a_{13} \\ a_{21} & a_{22} & 0 \\ 0 & a_{32} & a_{33} \end{bmatrix} \tag{6.18}$$

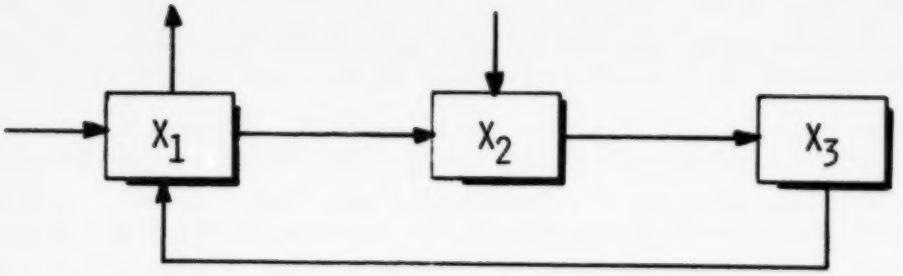


Figure 9. Hypothetical compartment system.

Assume the two exogenous inputs u_1 and u_2 drive the system to a steady-state, resulting in the following equation of the form of (6.12):

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} a_{11} & 0 & a_{13} \\ a_{21} & a_{22} & 0 \\ 0 & a_{32} & a_{32} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}. \tag{6.19}$$

Performing $m=2$ experiments with two linearly independent constant inputs generates the ensemble of steady-states given by (6.5) as

$$\begin{bmatrix} a_{11} & 0 & a_{13} \\ a_{21} & a_{22} & 0 \\ 0 & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix} = - \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \\ 0 & 0 \end{bmatrix}. \tag{6.20}$$

Taking the transpose of each side yields

$$\begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \end{bmatrix} \begin{bmatrix} a_{11} & a_{21} & 0 \\ 0 & a_{22} & a_{32} \\ a_{13} & 0 & a_{33} \end{bmatrix} = - \begin{bmatrix} u_{11} & u_{21} & 0 \\ u_{12} & u_{32} & 0 \end{bmatrix} \tag{6.21}$$

which is the matrix form of the following three sets of equations in the six unknown rate coefficients:

$$\left.\begin{aligned} x_{11}\ a_{11} + x_{31}\ a_{13} &= -u_{11} \\ x_{12}\ a_{11} + x_{32}\ a_{13} &= -u_{12} \end{aligned}\right\} \qquad (6.22)$$

for the first column of $\underline{A}$,

$$\left.\begin{aligned} x_{11}\ a_{21} + x_{21}\ a_{22} &= -u_{21} \\ x_{12}\ a_{21} + x_{22}\ a_{22} &= -u_{22} \end{aligned}\right\} \qquad (6.23)$$

for the second column, and

$$\left.\begin{aligned} x_{21}\ a_{32} + x_{31}\ a_{33} &= 0 \\ x_{22}\ a_{32} + x_{32}\ a_{33} &= 0 \end{aligned}\right\} \qquad (6.24)$$

for the third column.

The system of Figure 9 may be tested for identifiability by inspecting the necessary conditions provided in this section. There is a path from some input to every compartment and one outlet to the environment is reachable from every compartment, thus satisfying Theorems 6.1 and 6.2. The system has two exogenous inputs and at most one (m-1) endogenous input to a single compartment. Notice that the sets of equations (6.22) and (6.23) have a unique solution if and only if

$$\begin{vmatrix} x_{11} & x_{31} \\ x_{12} & x_{32} \end{vmatrix} \neq 0 \quad \text{and} \quad \begin{vmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \end{vmatrix} \neq 0. \qquad (6.25)$$

Furthermore, equation (6.24) has a nontrivial solution if and only if

$$\begin{vmatrix} x_{21} & x_{31} \\ x_{22} & x_{32} \end{vmatrix} = 0.$$

These conditions are required for identifiability and are obtained when the $\underline{X}$-matrix of steady-states has row rank of m=2 and the individual state vectors can lie anywhere in the m-dimensional subspace of the state space R^n. A sufficient condition for these constraints on the $\underline{X}$-matrix of steady-states is provided by the controllability of $(\underline{A}, \underline{B})$.

Equation (6.22), (6.23) and (6.24) can provide five independent equations in the six unknown entries in the $\underline{A}$-matrix. Thus, with this example, it is clear that knowledge of the turnover a_{33} of compartment 3, or the exogenous flow $(a_{33})x_3$ from compartment 3 provides the identification of the systems model. It is also clear that closure of compartment 3 gives

$$a_{13} + a_{33} = 0, \tag{6.27}$$

which along with equations (6.22) and (6.23) and one equation drawn from (6.24) defines six independent equations in the six unknown entires in $\underline{A}$.

If the compartment(s) without an exogenous input is (are) not closed, it may be difficult, if not impossible, to identify the compartment model from steady-state measurements alone. In such cases, it may be useful to define the maximum identifiable sub-model of the system. The identifiable sub-model parameter matrix $\underline{A}_{max}$ consists of all transfers associated only with compartments which are either closed or have exogenous inputs. The dimension of the sub-model is (m+c) where c is equal to the number of compartments without an input or a flow to the environment. For example, consider the system of Figure 9 with an additional flow from compartment 3 to the environment. The matrix of rate, coefficients for maximum identifiable sub-model is

$$A_{max} = \begin{bmatrix} a_{11} & 0 \\ a_{21} & a_{22} \end{bmatrix}. \tag{6.28}$$

The identifiability of this sub-model depends only on the measurement of steady-states. In order to identify the full system model an experimental design which incorporates material flow measurements must be implemented.

As a practical matter, it is often true that the closure of a compartment indicates its inaccessability with respect to exogenous inputs. Thus, the case when (m+c) = n is important in the applications of the theory of structural identifiability. For this case the following theorem gives sufficient conditions for identifiability.

Theorem 6.4

An open compartment model with m inputs is identifiable provided:

1. The pair ($\underline{A}$, $\underline{B}$) is controllable.
2. A maximum of (m-1) endogenous inputs enter each of the n compartments.
3. The (n-m) compartments without exogenous inputs are closed.

Proof:

Because ($\underline{A}$, $\underline{B}$) is controllable, the row rank of $\underline{X}^T$ is m, and

$$\underline{X}^T \underline{a}_k = \underline{z}_k \qquad k=1, 2, \ldots, m \tag{6.29}$$

has a unique solution for the m^2 unknowns in the n-vectors $\underline{a}_k$. Also, the controllability of ($\underline{A}$, $\underline{B}$) along with the fact that $\underline{A}$ is open implies that

$$\underline{X}^T \underline{a}_{k+m} = \underline{0} \qquad k=1, 2, \ldots, c \tag{6.30}$$

where c=n-m, gives c(m-1) equations in cm unknowns. These results follow from the fact that controllability implies an input to (6.1) can produce an arbitrary steady-state which is not constrained to lie in a proper subspace of R^n. Also, since $\underline{A}$ is open without closed proper subsystems, the resultant coeffic-

ient matrix [see (6.24)] of (6.30) is of rank (m-1). So, equations (6.29) and (6.30) give

$$m^2 + c(m-1) = mn-c \tag{6.31}$$

independent equations in nm unknowns. However, c compartments are closed, yielding c independent equations for the columns of $\underline{A}$. Thus, the solution of the resultant set of mn linearly independent equations gives the desired nm rate coefficients comprising the $\underline{A}$-matrix.

Now consider the case in which some states cannot be measured directly. It will be shown by example that it is impossible to identify all unknown parameters unless there is access to every compartment. Assume that steady-state measurements can be taken only from compartments 1 and 2 of Figure 9. The ensemble measurement matrix $\underline{Y}$ may be given by

$$\underline{Y} = \underline{C}\,\underline{X} \tag{6.32}$$

where C is defined by equation (5.2), resulting in

$$\begin{bmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \end{bmatrix} \tag{6.33}$$

substituting the measured values $\underline{Y}$ into the system of equation (6.20) gives the system

$$\left.\begin{aligned} y_{11}\,a_{11} + x_{31}\,a_{13} &= -u_{11} \\ y_{11}\,a_{21} + y_{21}\,a_{22} &= -u_{21} \\ y_{21}\,a_{21} + x_{31}\,a_{33} &= 0 \\ y_{12}\,a_{11} + x_{32}\,a_{13} &= -u_{12} \\ y_{12}\,a_{21} + y_{22}\,a_{22} &= -u_{22} \end{aligned}\right\} \tag{6.34}$$

with the additional equation $a_{13} + a_{33} = 0$ provided by equation (6.24). Notice that the result is a set of six linearly independent equations with eight unknowns since the values of x_{31} and x_{32} cannot be measured.

Although the parameters associated with compartments which are immeasurable cannot be estimated, again, a maximum sub-model can be identified. The identifiable sub-model flow matrix is composed of those parameters associated only with those compartments which can be measured directly and satisfy conditions given when all states are measurable. Thus, for Figure 9, the maximum identifiable sub-model flow matrix $\underline{A}_{max}$ is that of (6.25).

Controllability of the system (6.1) allows the exogenous inputs to produce arbitrary steady-state values anywhere in state space resulting in

sufficient, but not necessary, conditions for the structural identifiability of the system when direct measurements can be obtained from every compartment. There is, however, no need to investigate the observability of the system as this concept plays no role in solving the problems of constant infusion identifiability.

Although the conclusions on identifiability for the constant infusion method are somewhat limited by system structure and the lack of necessary conditions, it should be pointed out that the prevalent notion that "identification of dynamic parameters on the basis of measurements is only possible if the measurements are taken when the system is in a transient state" (Graupe, 1976, p. 7) is erroneous, because complete sets of parameters can be identified when a system is in steady-state under conditions which are often met in practice.

SECTION 7

EXPERIMENTAL DESIGN

The experimental design for microcosms receiving toxic material inputs developed by this research project focuses upon deciding what can be measured and what models support the measured data. The basic design requires pre-experiment measurements in order to determine the parameters of the Mulholland-Gowdy sampling theory for system identification and modeling. Some idea of the time scale of the system must be obtained for a useful definition of the flows and material transfers between compartments. Of course, the number of compartments in the system should be discerned as a first step.

The Mulholland-Gowdy sampling theory requires estimates for the maximum compartmental turnover and the minimum exogenous transfer rate. The maximum turnover describes how fast the toxic material moves from one compartment to another, while the minimum exogenous turnover bounds the toxicant degradation rate for each compartment. Pre-experiment measurements are also needed to establish the precision of the measured data, e.g., the number of significant digits in the data output of the laboratory measuring equipment. The periodic sampling interval τ for time series state data collection resulting from a basic experiment, as described by Table 1(e), is then defined by (3.4) and (3.6).

Many diagnostic inputs, of the form of basic experiments (Table 1), are required to perturb the laboratory system in order to elicit the transient state response required for data collection and system identification. Thus, the basis for the experimental design is a diagnostic input of the form shown in Figure 10. It is assumed the laboratory system is of a flow-through type, open to its environment, so that a constant inflow of toxic material u_o applied to the natural microcosm inputs establishes a steady-state. This initial system steady-state is observed by noting the constant levels of toxin within each compartment. The inflow u_o is a chronic level of toxin carefully chosen to have minimal effects on the biota. The time required to establish the initial steady-state x_o response to u_o is approximately equal to six (6) time constants, obtained by multiplying the reciprocal of the minimum exogenous turnover by six (6). Assuming the flow-through process takes place at a rate greater than degradation, the settling time estimate produces $6/\delta$, which essentially accounts for the exponential behavior of degradation in the transient state. At time T_1 the input u_o is reduced by Δu, where

$$u_1 = u_o - \Delta u, \tag{7.1}$$

so that the microcosm seeks a new steady-state x_1. In order to identify a

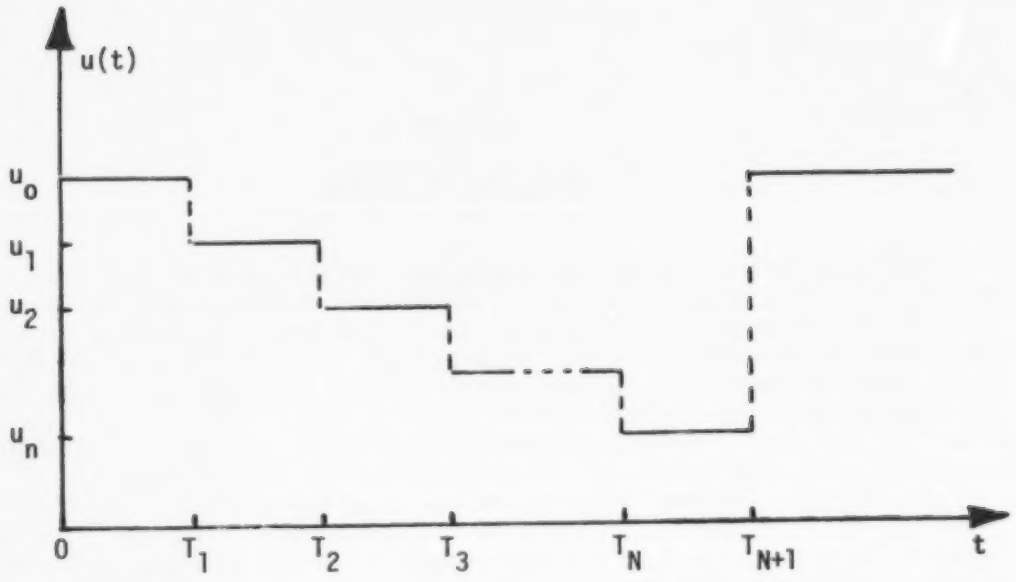


Figure 10. Diagnostic input for experimental design.

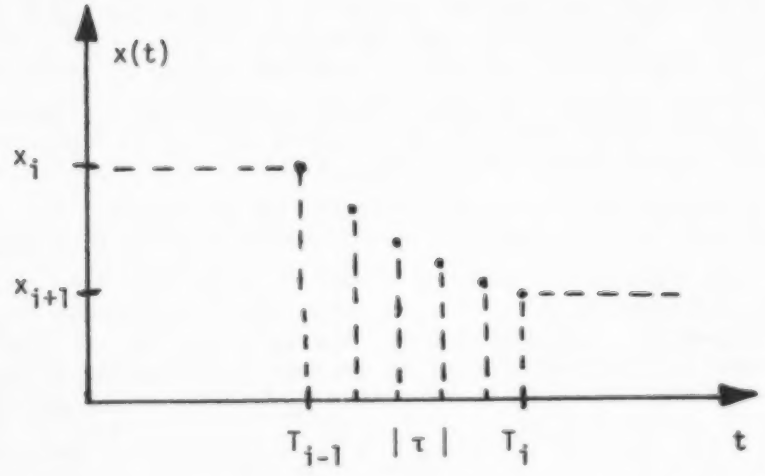


Figure 11. Response to diagnostic input for experimental design.

linear model for the laboratory ecosystem, n samples of the transient state must be resolved between the steady-states x_0 and x_1. Thus, the input change Δu must be large enough to produce this amplitude resolution. For linear compartment models, equation (3.2) prescribes that the transient state x(t) is bounded by

$$x(t) \geq x_1 + (x_0 - x_1)e^{-\alpha t}. \tag{7.2}$$

Linear system theory also gives

$$(u_0/u_1) = (x_0/x_1), \tag{7.3}$$

and since

$$x_1 = x_0 - \Delta x \tag{7.4}$$

it is easily shown that (7.1), (7.3) and (7.4) combine to give

$$\Delta x = (x_0/u_0)\, \Delta u. \tag{7.5}$$

Assuming a sampling period of τ, it is clear that $x(n\tau)$, the n-th sample taken after T_1, must be different than x_1, i.e.,

$$x(n\tau) > x_1 + 10^{-d} \tag{7.6}$$

within the finite arithmetic precision of the measurements. Thus, equation (7.2) gives

$$\Delta x e^{-\alpha n\tau} > 10^{-d} \tag{7.7}$$

and a lower bound for Δu results by substituting (7.5) into (7.7):

$$\Delta u > (u_0/x_0)\, e^{-\alpha n\tau}\, 10^{-d}. \tag{7.8}$$

This process is continued through time T_N resulting in enough measured data to construct N (local) linear models for ecosystem structure and function. Since only positive inflows of toxic material are possible

$$N\Delta u < u_0 \tag{7.9}$$

must hold true. Hence, an upper bound on Δu is obtained

$$\Delta u < u_0/N. \tag{7.10}$$

In response to the staircase diagnostic input of Figure 10, at least n samples of the microcosm state are measured with a sampling interval of τ. As in Figure 11, the time difference $(T_{i+1} - T_i)$ during which the transient state response is observed must be greater than six (6) time constants, i.e.,

$$T_{i+1} - T_i \geq 6/\delta \tag{7.11}$$

to insure the system is in steady-state before the next input transition takes place.

The Mulholland-Gowdy sampling theory has been used to design an experiment for studying laboratory ecosystems. Experimental design parameters (α, δ, d, etc.) can all be obtained from pre-experiments involving the microcosm or its isolated components. The result of an experiment based upon the diagnostic input of Figure 10 is a data set which is capable of constructing a series of (local) linear models for the microcosm. Furthermore, the validity of these linear models can be tested using the measured data. Two tests exist for model validation. First, for linear models, the input level ratios must equal their respective steady-state response level ratios:

$$u_{i+1}/u_i = x_{i+1}/x_i \tag{7.12}$$

for all i = 0, 1, ..., N. Of course, practical laboratory experiments will result in statistical estimates for these steady-states, and standard statistical tests can be used to determine the validity of (7.12). The second test is qualitative, noting that linear compartment models produce monotone transition states in response to basic experiments in which transfers between steady-states are observed. If the samples of the microcosm state during any $(T_{i+1} - T_i)$ time period do not decrease monotonically from steady-state x_i to x_{i+1}, then the linear compartment modeling hypothesis is incorrect. Probably all microcosms will fail this test for linearity when Δu is too large. Thus, local behavior of the system and the ability to describe this behavior by linear models are believed to be related.

The validity of the experimental design, as based upon the linear compartment modeling objective, depends upon the equality of the steady-state ratios and the monotonic behavior of the transition between steady-states. When these validation tests fail, the microcosm modeling objective must be based upon nonlinear system theory.

If a great deal of intuition exists regarding the microcosm processes, then it may be possible to characterize these processes mathematically within a nonlinear model of known structure. In terms of the general concepts of systems theory, it is extremely difficult to identify nonlinear models using transient state data. The technique presented in Section 3 of this report applies only to linear systems and because it relies on a general solution for the linear model, the scheme cannot be generalized to nonlinear identification. However, another approach for obtaining the parameters of a nonlinear model of known structure is possible using only steady-state measurements.

The proposed method of nonlinear steady-state model identification is best illustrated by example. Consider the very elementary single compartment system with input u and state x. From pre-experiment observations, scientific intuition, or theoretical constructs regarding the microcosm processes, the structure for the model is assumed to be of the form

$$\dot{x} = -ax + bx^2 + u \tag{7.13}$$

where a and b are unknown parameters which characterize the model structure to the particular ecological processes. For b = 0 the system is linear and the parameter a is the compartmental turnover. The identification of the parameters a and b proceeds as follows. Let a constant input u_1 be applied to the

system, which results in a steady-state x_1 being observed. Then another constant input $u_2 \neq u_1$ is applied, and its corresponding steady-state x_2 is also observed. Substituting these steady-states into (7.13), while noting that a steady-state is defined by the time derivative of x being identically zero, two simultaneous algebraic equations result:

$$\begin{aligned} 0 &= -ax_1 + bx_1^2 + u_1 \\ 0 &= -ax_2 + bx_2^2 + u_2. \end{aligned} \tag{7.14}$$

Because the inputs and states are measured, and hence known, equation (7.14) represents two linear algebraic equations in the unknowns a and b. Furthermore, a unique solution of (7.14) for a and b exists if and only if $x_1 \neq x_2$. Thus, a model of known structure can be identified from steady-state measurements. However, since an infinite number of nonlinear models could fit the steady-state data, either confidence in the model structure must be present or some validation scheme for the model is required.

To demonstrate the multiplicity of nonlinear models which can be identified from a fixed steady-state data set, consider the model structure:

$$\dot{x} = -cx + dx^k + u \tag{7.15}$$

where c and d are unknown parameters and $k > 3$ is any integer. The same steady-state data set used for identifying (7.13) now gives

$$\begin{aligned} 0 &= -cx_1 + dx_1^k + u_1 \\ 0 &= -cx_2 + dx_2^k + u_2 \end{aligned} \tag{7.16}$$

which for each fixed $k > 3$ yields a unique solution as long as $x_1 \neq x_2$. Some knowledge of the ecological process under study and its theoretical formulation could help to decide which model structure best represents the system. Also, each model structure could be compared with time series data for the transient response of the system in order to decide the best model fit to the data.

The scheme presented for nonlinear identification of the parameters of models of known structure generalizes. For (7.13) the model consists of a single equation with two unknown parameters which are obtained from two steady state measurements. In general, a model consisting of n compartments and M unknown parameters requires N steady-states measurements, where

$$nN = M. \tag{7.17}$$

Thus, in Figure 10, the N levels in the diagnostic input provide a data set capable of determining $M = nN$ unknown parameters in a nonlinear model of known structure which represents a microcosm of n compartments. At time T_{N+1} a large (positive) step input is again applied to the system to re-establish the initial state. The time series which results from this step input is of use

in validation of the assumed nonlinear model structure.

To complete the nonlinear analysis, it should be noted that the N (local) linear models which result from the diagnostic staircase input can be used to compute the material flows between each compartment as they depend upon the compartment levels. Such tables of global measurements of ecological structure and function have been used by Smith (1970) to identify the model structure for an ecosystem. Thus, it may be possible to use the local models to validate the nonlinear model structure, and by doing so provide an important connection between the linear and nonlinear model identification methods.

A pre-experiment to determine the parameters of the Mulholland-Gowdy sampling theory has been run at the Environmental Research Laboratory in Athens, Georgia, for a microcosm consisting of water, algae, snails and sediment compartments. A slug of radiolabelled methoxychlor was introduced into the water of the laboratory ecosystem. Samples of the toxin and radioactivity were obtained in order to determine estimates for degradation and compartmental transfers. These estimates define α and δ, the maximum turnover and minimum exogenous turnover. By analyzing the methoxychlor samples, some idea of the arithmetic precision of the data is obtained. All of these estimates for the sampling theory parameters determine an experimental design, based upon the diagnostic input of Figure 10, for the particular microcosm under study. It is hoped the experimental design will be tested in the laboratory sometime in the future.

SECTION 8

COMPUTER PROGRAM

A digital computer user package implementing the compartment model identification algorithm has been developed. Programmed in standard FORTRAN, the code which implements the identification algorithm is available in two forms, batch and interactive, both of which run efficiently on a standard IBM 370 operating system. The code is independent of any special library routines, and as such is completely transportable to any IBM System/360 or System/370 series computer. The interactive program can be implemented on any IBM System/370 time share operating system (TSO).

The software consists of a main program and one subroutine, EIVECT, the flow diagrams of which are shown in Figures 12 and 13.

The program begins by reading the number N of compartments in the biological system being analyzed, the number K of measurements obtained from a single experiment, and the pre-calculated sample period T. Two flags are then set which indicate row or column data input and printing options, respectively. The program then moves immediately to a loop that reads and stores the sample data array in matrix form, i.e., $\underline{X}(t)$. Since N+1 discrete measurements of the state are necessary and sufficient for the determination of the state transition matrix $\underline{\Phi}$, the program terminates for K < N+1. If K = N+1, two matrices of coefficients, $\underline{X}_1$ and $\underline{X}_2$, are formed from the N+1 state samples as described by (3.12) and (3.13). The solution for the state transition matrix $\underline{\Phi}$ is acquired by inverting matrix $\underline{X}_1$ of (3.12). Gaussian elimination with partial pivoting on a matrix scale is used. Upon computing the N x N matrix subroutine EIVECT is called for the identification of the matrix of rate coefficients $\underline{A}$. The indices I and L of the main flow diagram are utilized in the formation of a loop in which several $\underline{A}$ matrices may be computed for a comparative analysis if K > N+1.

Subroutine EIVECT solves (3.14) for the matrix of transfer constraints $\underline{A}$. The EISPACK (IBM/360 version by Smith, et al., 1976) is utilized to obtain the eigenvalues ω_i (i = 1, ..., N) and the eigenvectors of $\underline{\Phi}$. The EISPACK uses QR transformation and decomposition, an explanation of which is given by Wilkinson (1965) and Wilkinson and Reinsch (1971).

The matrix $\underline{\Phi}$ can be reduced to a diagonal matrix $\underline{\Omega}$ in which the eigenvalues ω_i (i = 1, ..., N) of $\underline{\Phi}$ appear on the diagonal. The eigenvalues λ_i (i = 1, ..., N) of $\underline{A}$ are determined by

$$\lambda_i = (1/T)\, \ell_n\, \omega_i, \tag{8.1}$$

and the reduced diagonal form $\underline{\Lambda}$ of the matrix of transfers $\underline{A}$ is formed. The matrix of rate coefficients is readily identified by

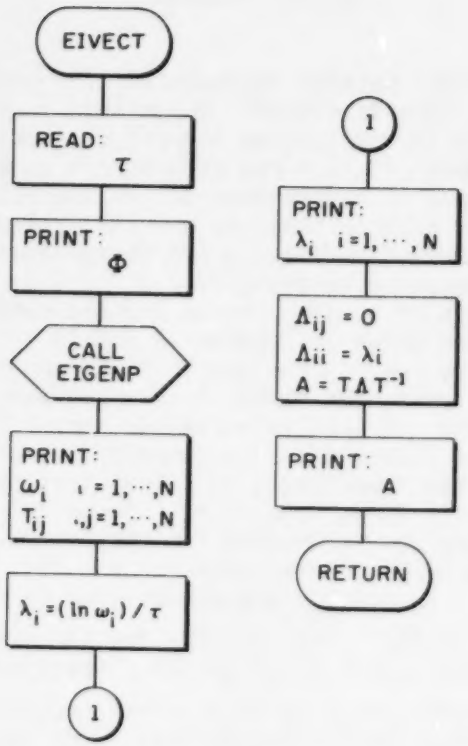


Figure 12. Flow chart for computer algorithm.

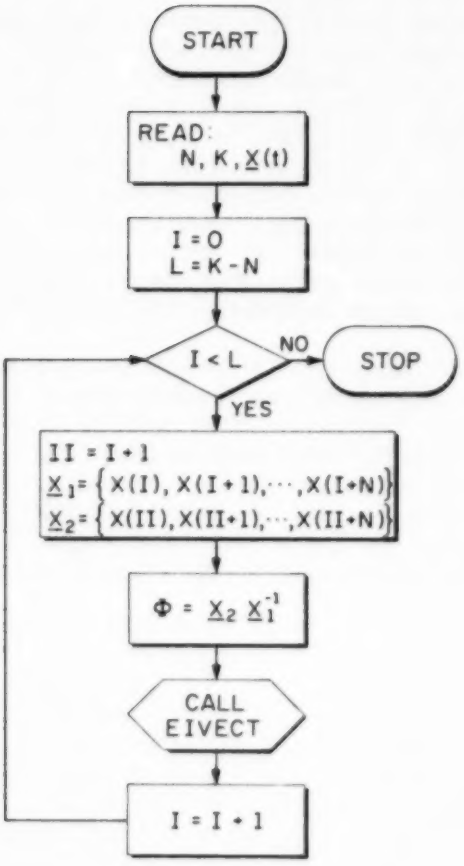


Figure 13. Flow chart for subroutine EIVECT.

$$\underline{S}^T \underline{A}^T = [\underline{S} \ \underline{\Lambda}]^T \qquad (8.2)$$

where $\underline{S}$ is a similarity transformation having the eigenvalues of $\underline{\Phi}$ as its column vectors. Equation (8.2) is solved successively for the columns of $\underline{A}^T$, again using Gaussian elimination. Note that the column vectors must be linearly independent for the existence of $\underline{S}^{-1}$. This follows from the assumption that the eigenvalues of $\underline{\Phi}$ are distinct.

It should be mentioned that EIVECT derives the complex matrix $\underline{A}$ for a real matrix $\underline{\Phi}$ using the complex principal value natural logarithm in (8.1). Also, all manipulations are in double precision. The input format for N, K and the two flags is I4, T is F10.0, and the state data is 8F10.0. The output is available in full double precision, but the current version of the program truncates to seven digits as given by 8D14.7 format.

The code, as submitted to the project officer, is well documented by comment cards, and the particular deck submitted will include data input cards for Smith's (1970) ecosystem model. An output from this deck, as run on the Oklahoma State University computer is included in the user package. A complete listing of the code which implements the identification algorithm is also in the user package.

The user package, as described, fulfills the grant obligations. However, because the interactive version of the program was of use to the researchers during the grant period, a listing of this code is also included. This listing indicates the changes which have been made to the batch program in order to implement it as an interactive program. Depending on the computer operating system, it is possible to load the batch program version as a data set and then edit it to conform to the interactive mode. This was the procedure used successfully by the researchers at Oklahoma State University.

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